UnityMol – SweetUnityMol

User Manual (Version Nov. 2014)

Installing the software

The software described below has been 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.

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

Documentation, input files, and series of illustrations can be found at

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

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

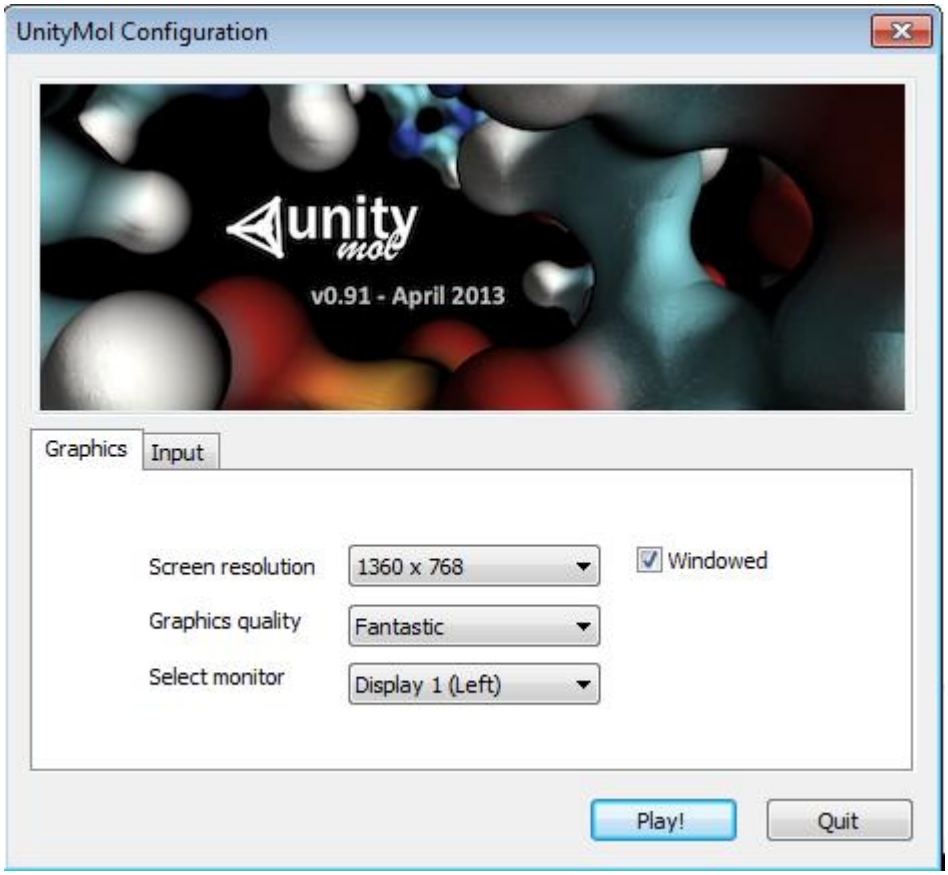
Mac version (date: 2014 10 02)

umol-macosx-universal-20141002.app

Linux version (data: 2014 10 02)

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

Running Windows version 32 and 64 bits



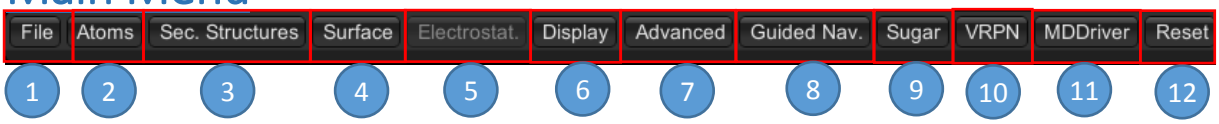
The shader needs OpenGl. Use the file **Run_SweetUmol_32.bat** or **Run_SweetUmol_64.bat** depending upon your version (the line has to look like "umol-winXX-20141002.exe –force-opengl".

DO NOT USE THE FULL SCREEN MODE (check "**Windowed"** in the "UnityMol Configuration" menu (this menu is the menu where you the resolution and click on "Play!").

Description of the coordinate input file (see Annex)

Ring Color Coding (see Annex)

Main Menu



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

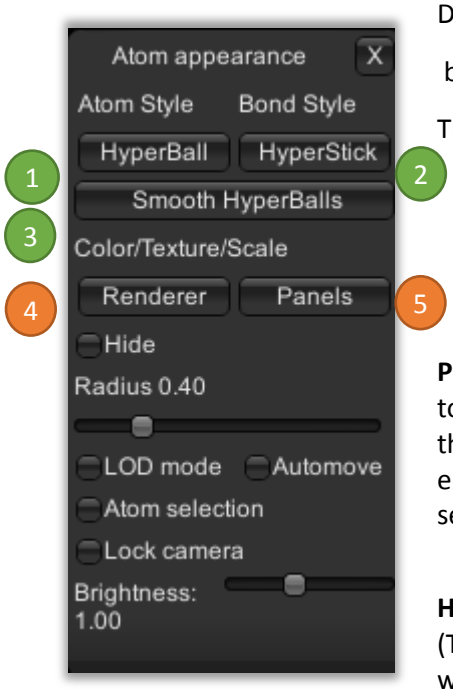
1 – File (PDB Loading)

1 – Open a file from hard drive (you can't change hard drive yet). **UnityMol and the pdb file have to be on the same drive but can be located on different directories)**.

2 – Fetch a pdb from the pdb database (*if "Proxy Server" and "Proxy Port" are filled, please remove all fields otherwise the program will crash*)

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.

2 – Atom

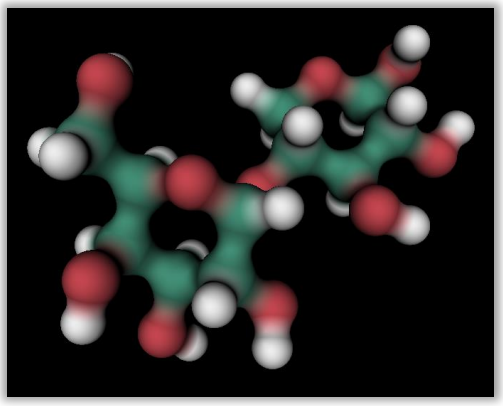


Different types of representations are available

by **Atom** or by **Bond.**

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

Hyperball Visualization



The **Renderer** and **Panels** 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.

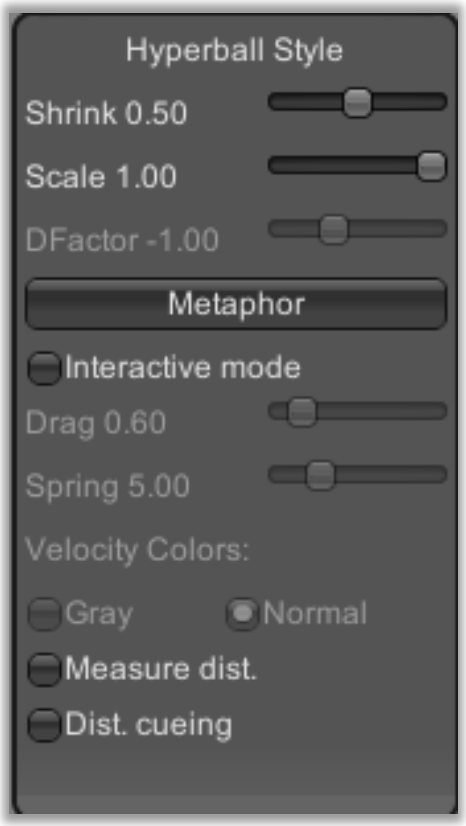
Radius: Change the radius of spheres.

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.

Brigtness: Adjust the brightness of Hyperballs.



A – HyperBall Style menu (3).

Shrink: To adjust the shape of the bond.

Scale: To adjust the scale of the bond.

DFactor: only for Biological Networks.

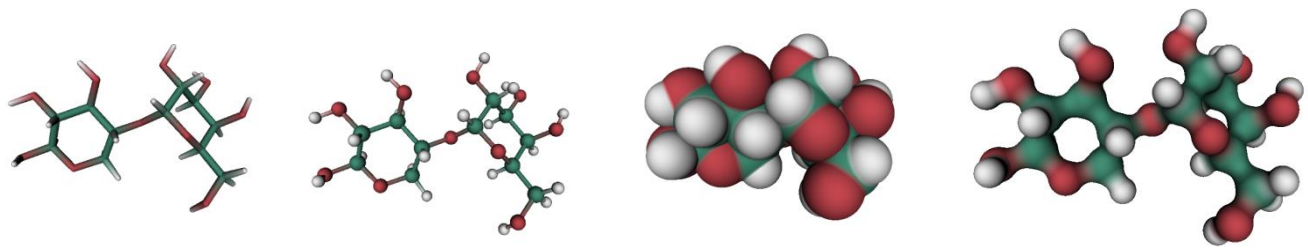
Metaphor: pre-configured style (CPK, Licorice, VdW, Smooth Hyperballs)

Interactive mode: use spring forces to make an interactive molecule (An atom can be dragged and he will go back to his original position).
Drag/Spring: spring parameters for interactive mode.
Velocity Colors: colors each atoms in interactive mode with the velocity of each one.

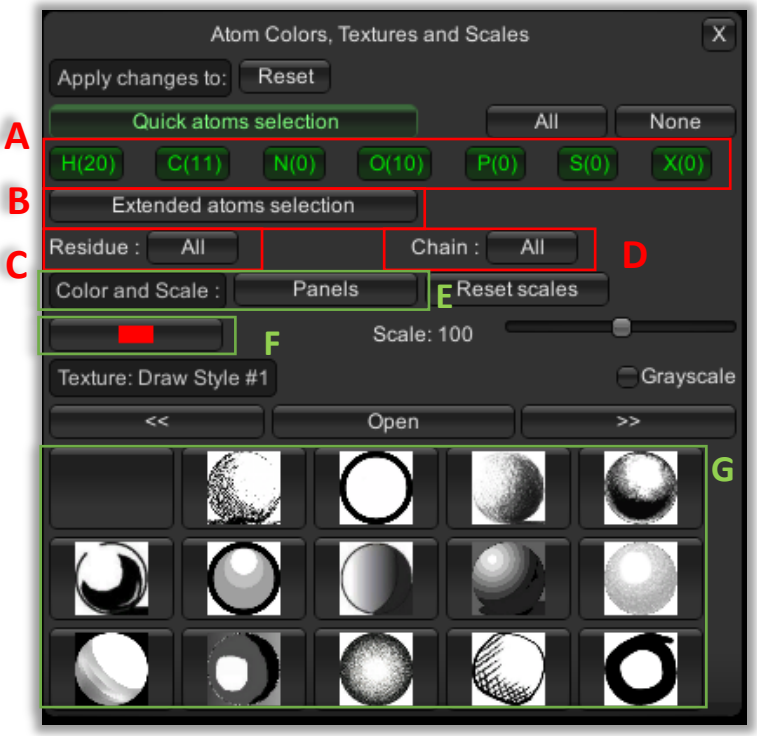
Measure dist: activate and click on 2 atoms to dispaly their distance.

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

Exemple Ball & Sticks, Licorice, VdW, Smooth Hyperballs



B - Rendered Menu (4)



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

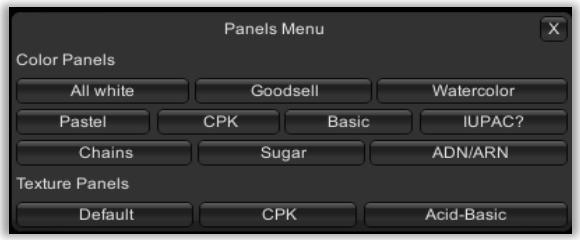
- Atom Type **(A)**
- Atom name **(B)**
- Residue name **(C)**
- By chain **(D)**

The selection can be combined.

Pre-configured coloration is on the **Panels** menu **(E)**. Another color can be 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 clickiging "**<<**" and "**>>**").

C – Panels Menu (3)



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

Color Panels:

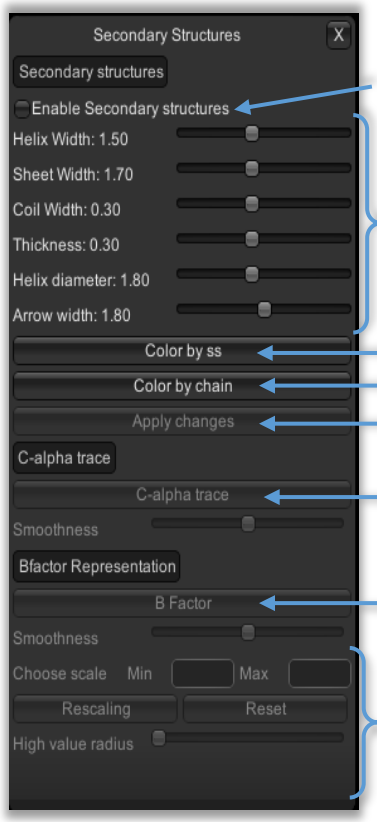
- **All white:** make the molecule all white.
- **Goodsell:** make the color softer.
- **WaterColor:** color carbons in blue.
- **Pastel:** default colors.
- **CPK**: color with the CPK color code.
- **Basic**: color carbon in green.
- **IUPAC**: color with the IUPAC color code.
- **Chains**: color by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



Activate the Secondary Structure visualization

Adjust parameters for the secondary structure visualization.

Color by secondary structure type.
Color by chain type

Don't forget to **click on this button to apply changes**.

Trace the shape of the proteins by a spline passing by all alpha carbons. Smoothness is used to adjust the visual aspect of the trace.

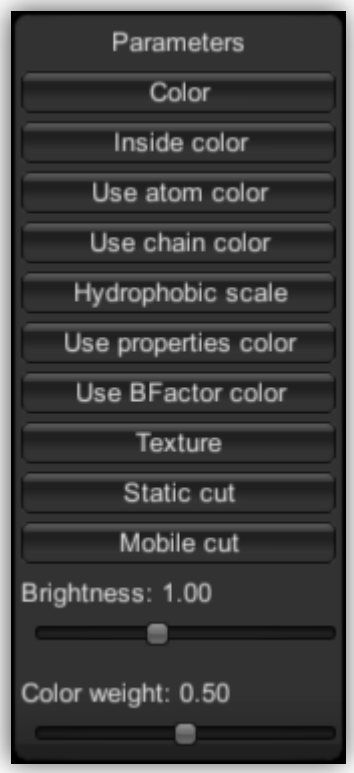
Like the C-alpha trace, but adjust the radius and the color of each sphere to the B factor value.

Adjust the scale of the B-factor used.

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, this 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 the same name) a file ".dx" and ".apf" generated with softwares such as APBS (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 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

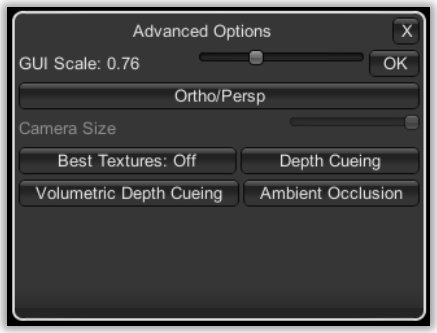
This menu is made to **take screenshot**, change the background and add special effects.
Screenshot (or P key): take a screenshot (prefer the P key or you will get all menus with the capture)
ScreenShot Sequence: doesn't work yet.
Background: add a picture in the background (switch between yes/no)
White/Gray/Black: 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
- **BLUR**: add a blur effect upon moving the camera.
- **NOISE**: add noise on the screen
- **BLUR2**: constant blur.
- **DOF**: focus on a point and make fuzzy all atoms away from this point This has to be used while being in the "Sphere" mode (Atoms -> Atom Style -> Sphere), and requires selecting (by clicking) an atom. Works better for large molecules.
- **CREASE**: doesn't work yet.
- **EDGE**: the edge of every atom is black.
- **VORTEX**: twist the molecule around the center.
- **GRAYS**: make the molecule black and white.
- **TWIRL**: similar to VORTEX
- **SEPIA**: use a SEPIA coloration.
- **GLOW**: make all atoms shiny.

7 – Advanced

This menu offers advanced options (only some are implemented)



GUI Scale: change the size of the GUI.
Ortho/Persp: doesn't work yet.

Best Textures: don't use anymore.

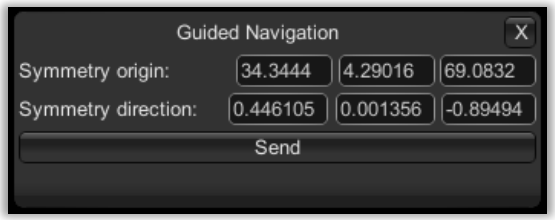
Depth Cueing: doesn't work yet.

Volumectric Depth Cueing: Doesn't work yet.

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

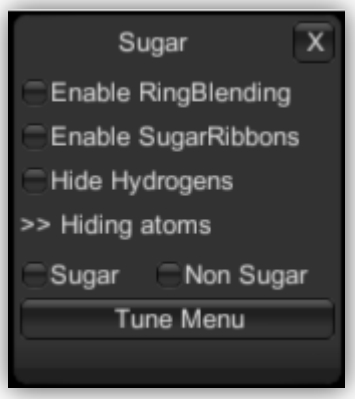
8 – Guided Navigation

This menu is used to make a "guided navigation", but for now it works only with the pdb 3EI0 (GLIC) as part of work in progress.



Symmetry origin: X,Y,Z coordinates of the center of symmetry.
Symmetry direction: vector of the symmetry direction.
Send: activate the guided navigation mode.

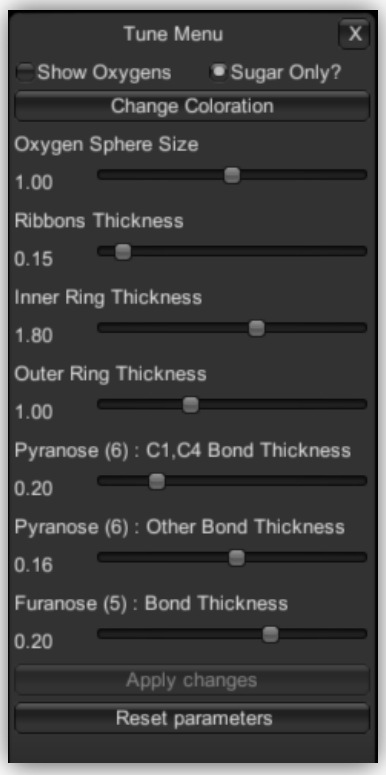
9 – Sugar



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.

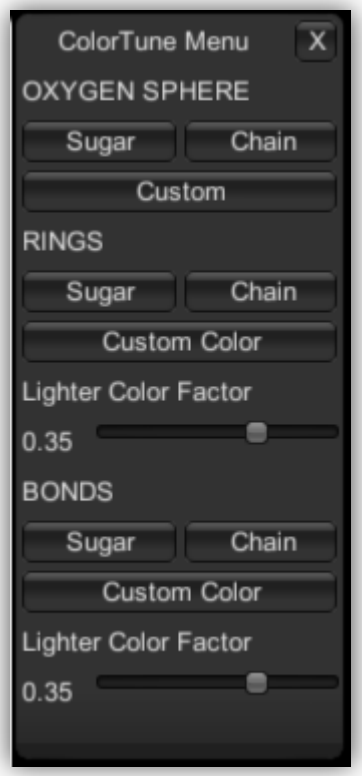
Tune Menu



Show Oxygens: to display the intracyclic oxygen atom as a sphere.
Sugar Only: apply the sugar Ribbons vizualisation 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.

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

Color Tune Menu



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**.

***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.

Binding Keys

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
X	Rotation LEFT
N	Rotation Right
B	ZOOM +
P	ZOOM –
P	Screenshot (only on local pdb)
BACKSPACE	Hide GUI
SPACE	Automove
R	Reset to center
C	Center to one or several atoms (select an atom with the selection mode).

Guided Navigation (only for 3EI0)

U	Constrained Navigation UP (panoramic mode)
J	Constrained Navigation DOWN (panoramic mode)
I	panoramic mode
Numpad + or B	Spreading chains
Numpad – or V	Narrowing chains
Numpad * or T	Reset chains

Format of the PDB File

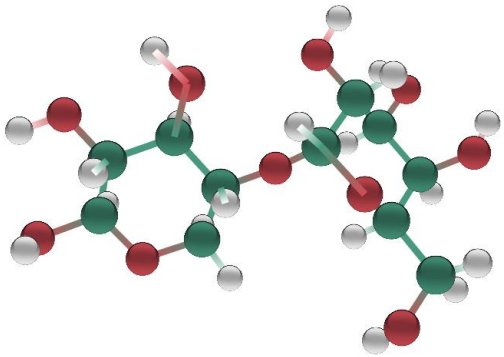
```
ATOM      1  C1  FUC     1       2.387 -19.488 -11.522  0.00  0.00  C1
ATOM      2  C2  FUC     1       3.248 -19.891 -12.734  0.00  0.00  C2
ATOM      3  C3  FUC     1       4.696 -19.417 -12.550  0.00  0.00  C3
ATOM      4  C4  FUC     1       5.229 -19.916 -11.196  0.00  0.00  C4
ATOM      5 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

Color code for monosaccharides

Monosaccharide	Code	Code Couleur
	A2G	
	AAL	
Abequose	**ABE**	
Aceose	**ACE**	
Aldotetrose	**ALT**	
Apicose	**API**	
Arabinose	**ARA**	
	BGC	
	BMA	
Acide Dehydroascorbique	**DHA**	
Fructose	**FRU**	
Fucose	**FUC**	
	FUL	
Galactose	**GAL**	
	GLB	
Glucose	**GLC**	
Gulose	**GUL**	
Idose	**IDO**	
Acide Ketodeoxynonulosonique	**KDN**	
Acide Ketodeoxyoctulosonique	**KDO**	
Manose	**MAN**	
	MMA	
	NAG	
Acide neuraminique N-glycolyl	**NEG**	
	NDG	
	NGA	
Rhamnose	**RHA**	
Ribose	**RIB**	
Acide Sialique	**SIA**	
Tagatose	**TAG**	
Talose	**TAL**	
Xylose	**XYL**	

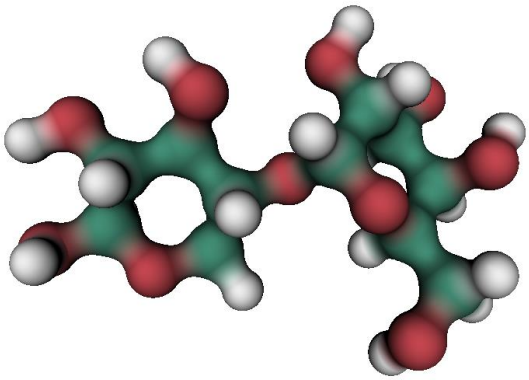
Examples

Particles mode.

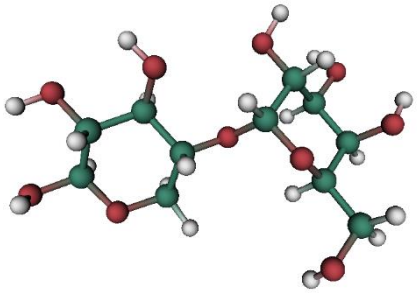


Smooth HyperBalls mode

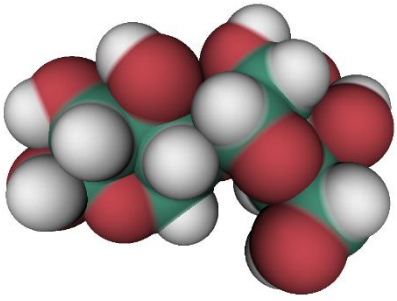
Default Smooth HyperBalls mode



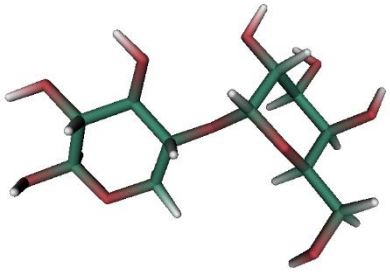
CPK



Wan Der Waals

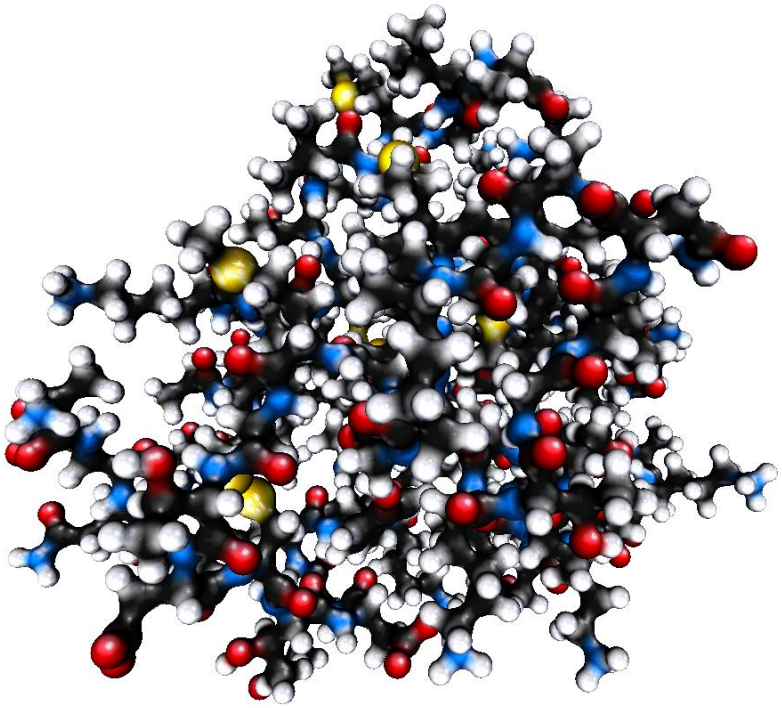


Licorice

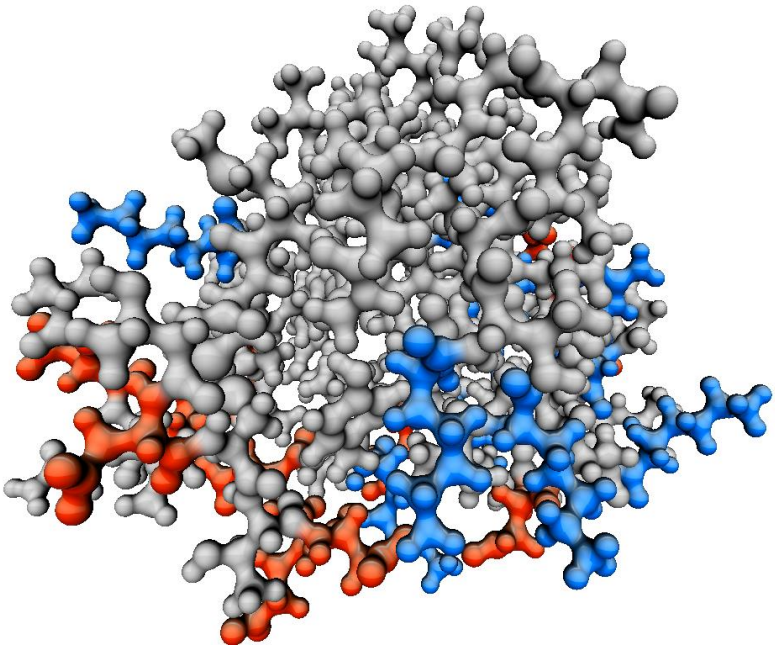


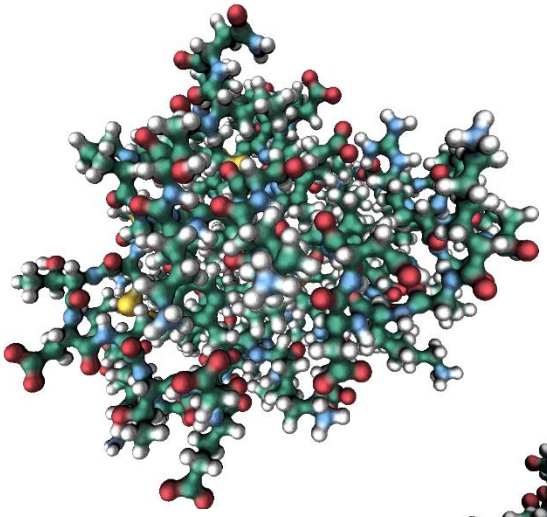
Texture

CPK

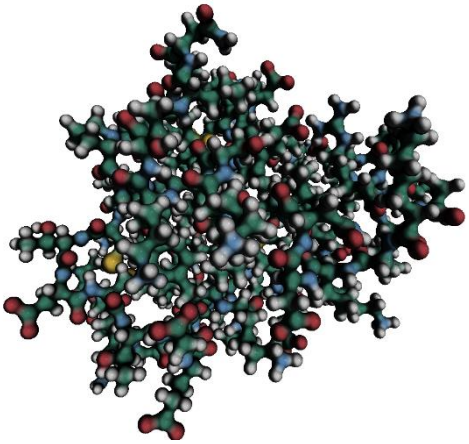


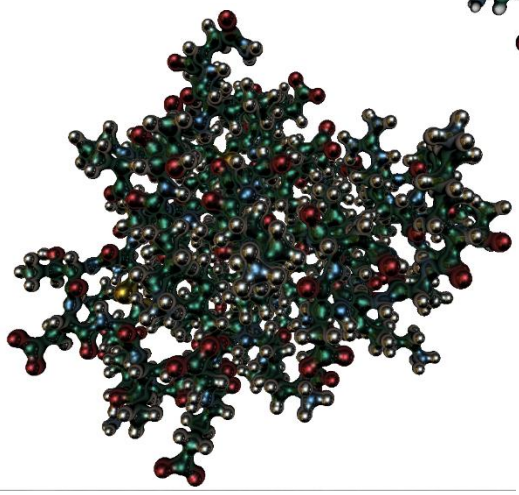
Acid-Basic





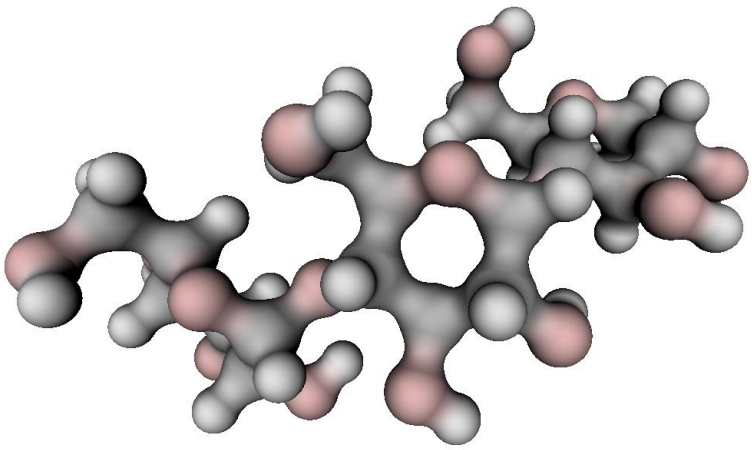
Other examples (Renderer Menu)



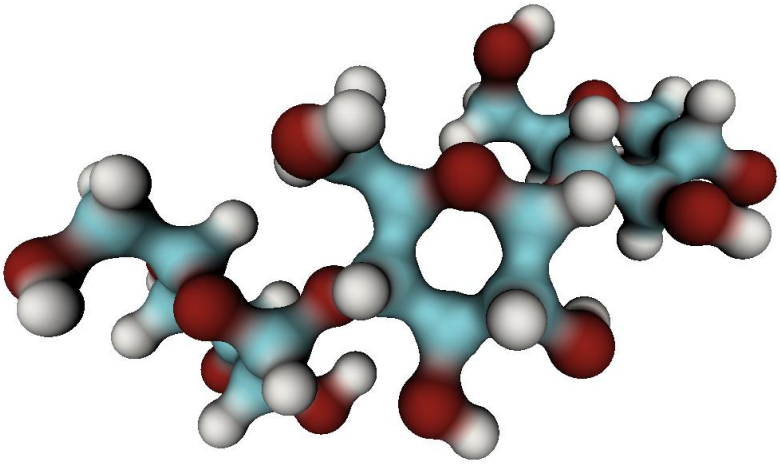


Coloration Mode

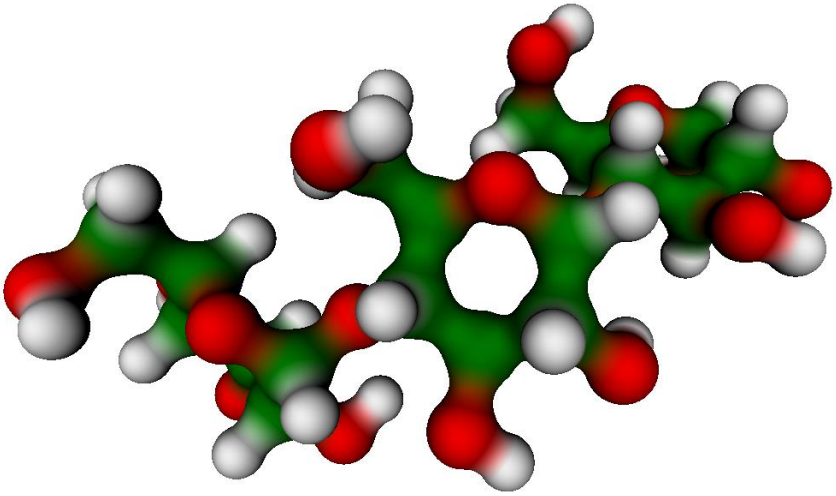
GoodSell



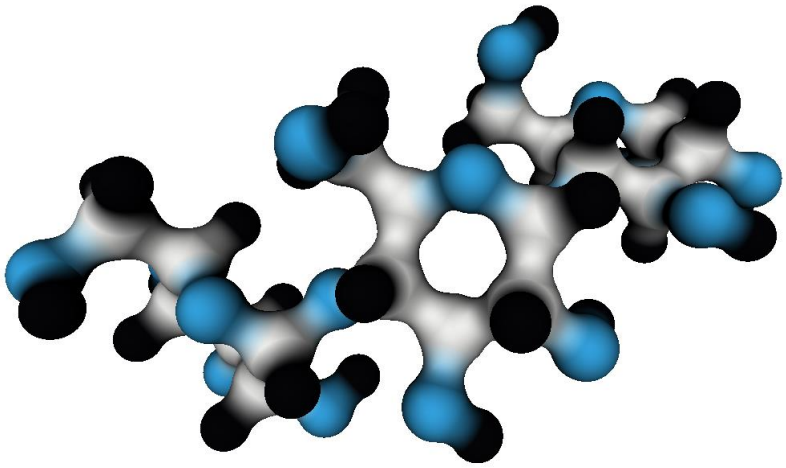
WaterColor



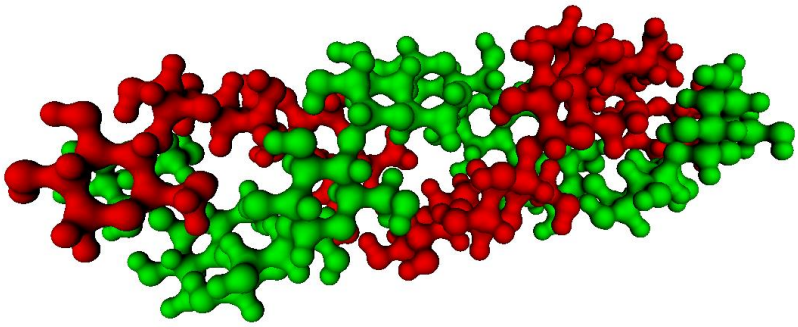
Basic



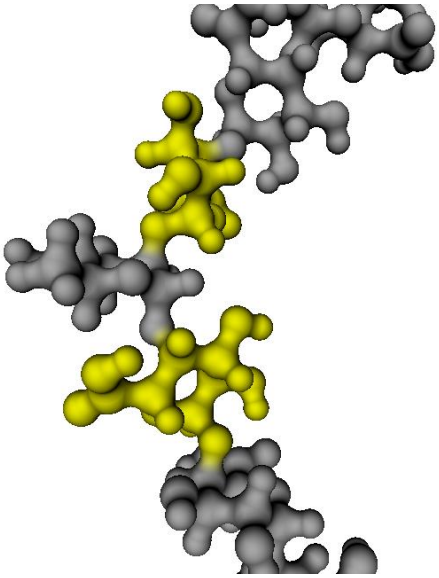
IUPAC



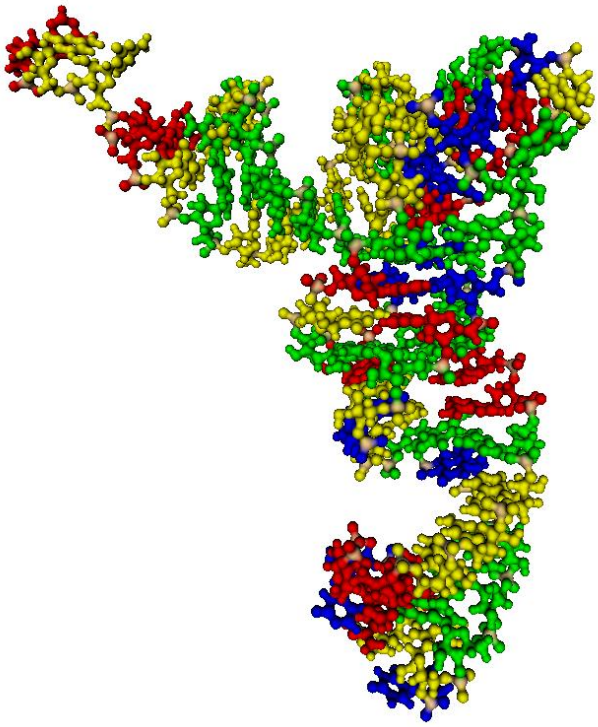
Chain



Sugar

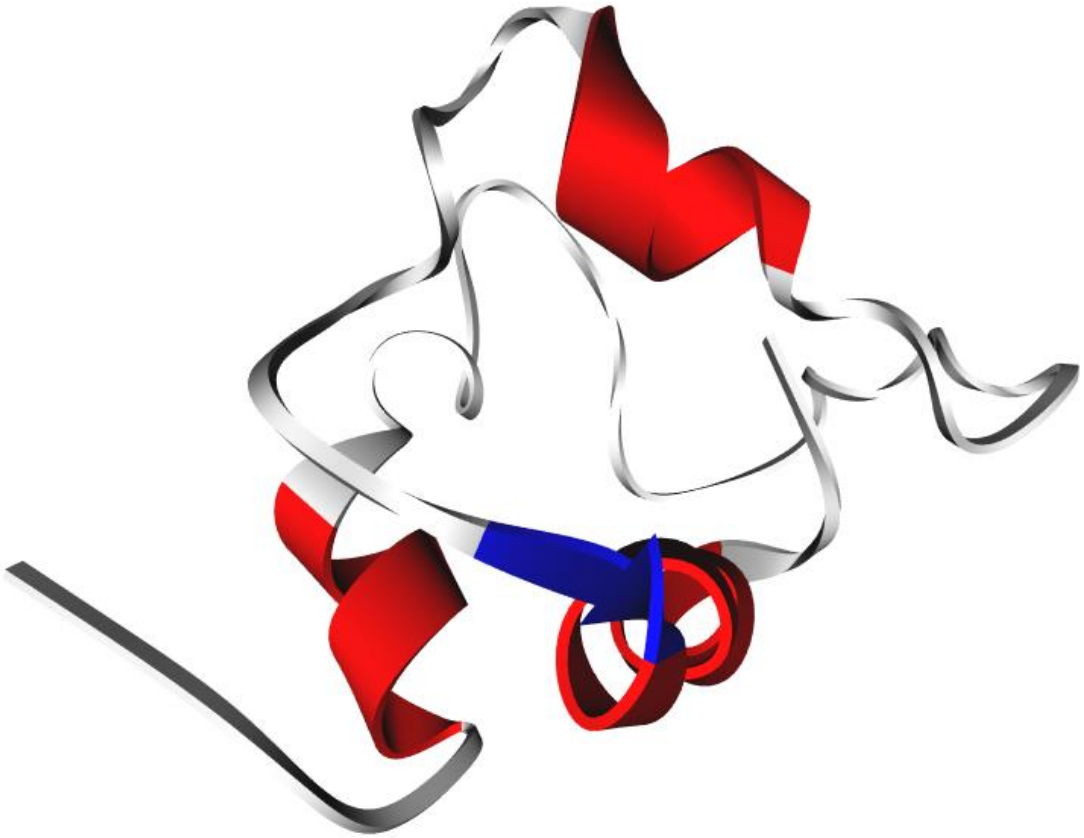


DNA/RNA

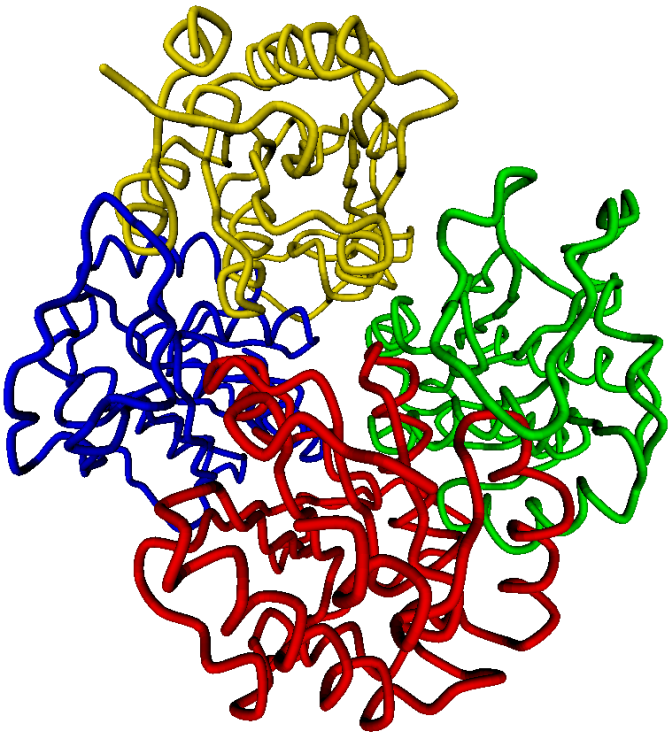


Secondary Structure Menu

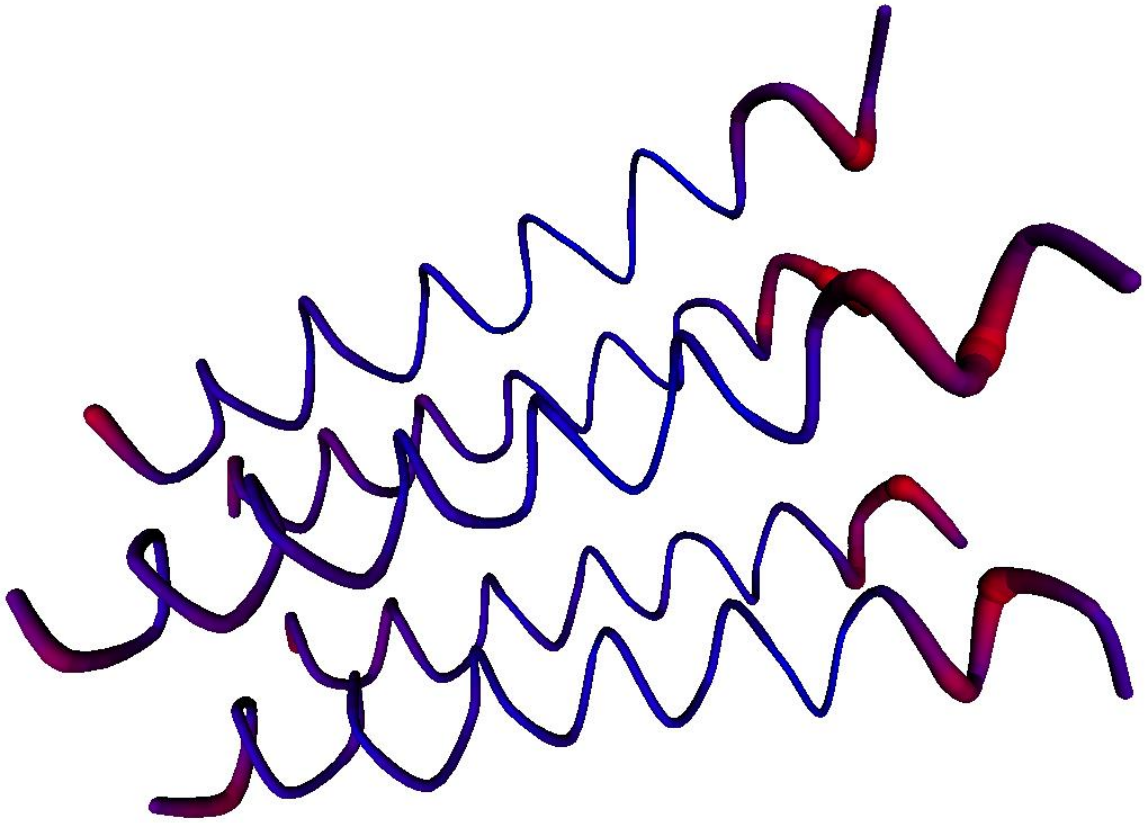
Secondary Structure



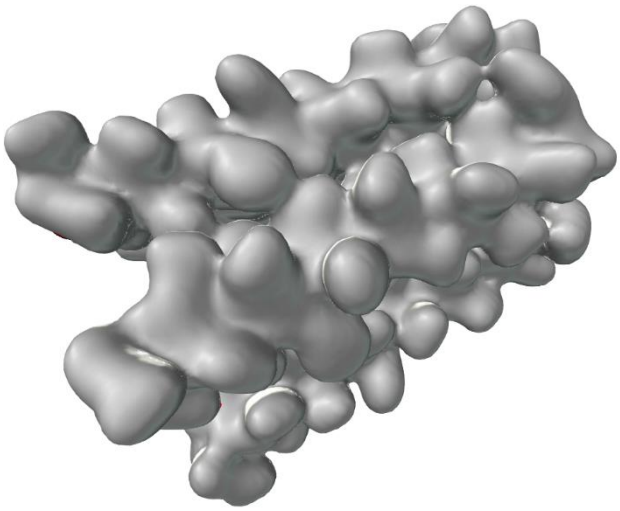
Ca-Trace



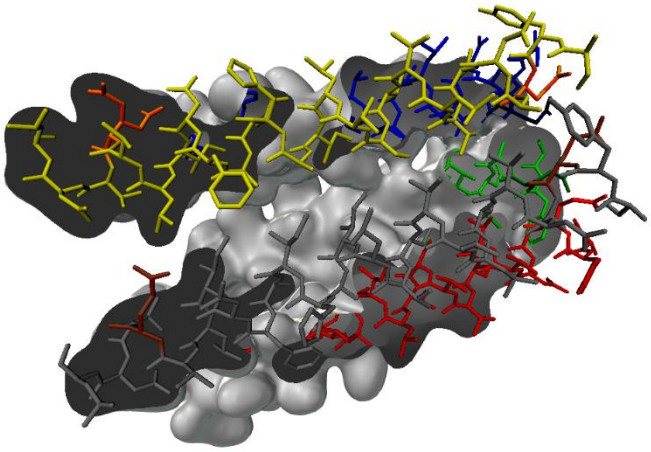
B-factor



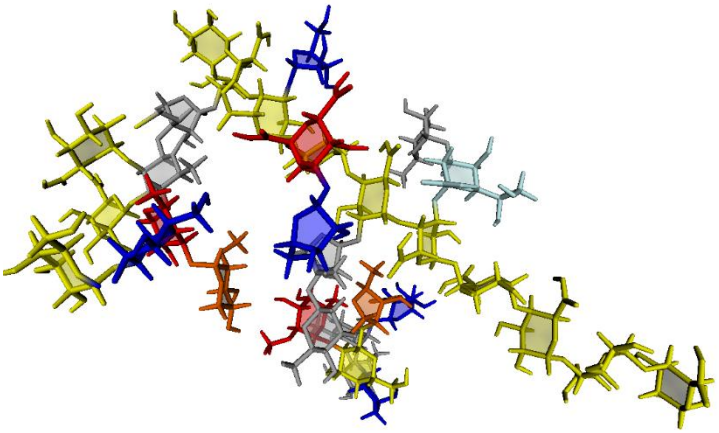
Surface Mode



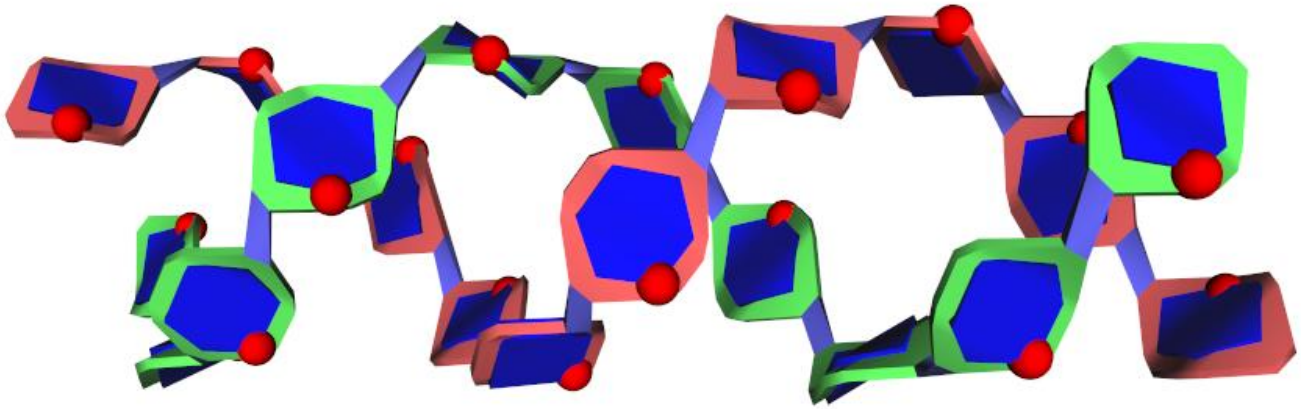
Surface with static/mobile Cut



Ring Blending (with sugar coloration)

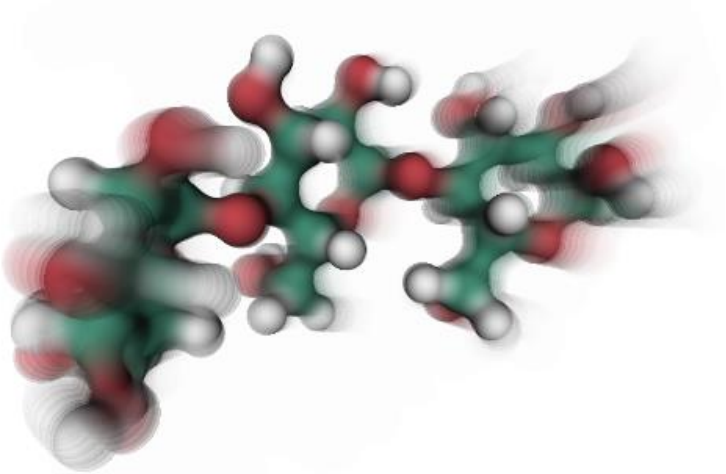


SugarRibbons

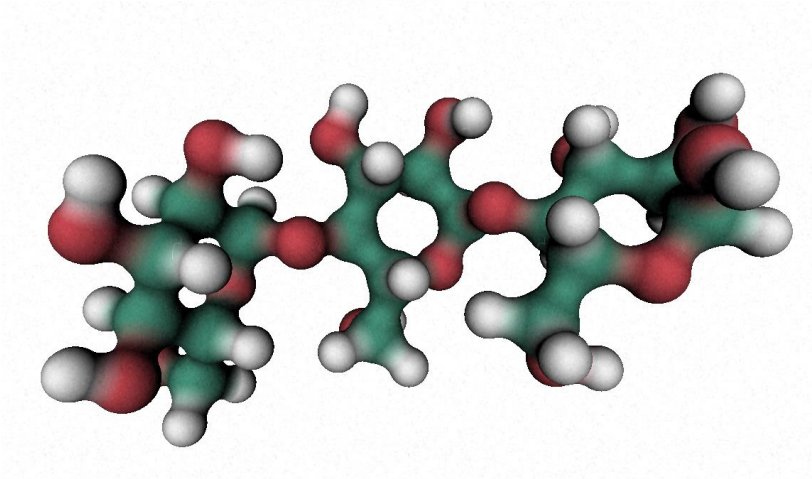


Special Effect

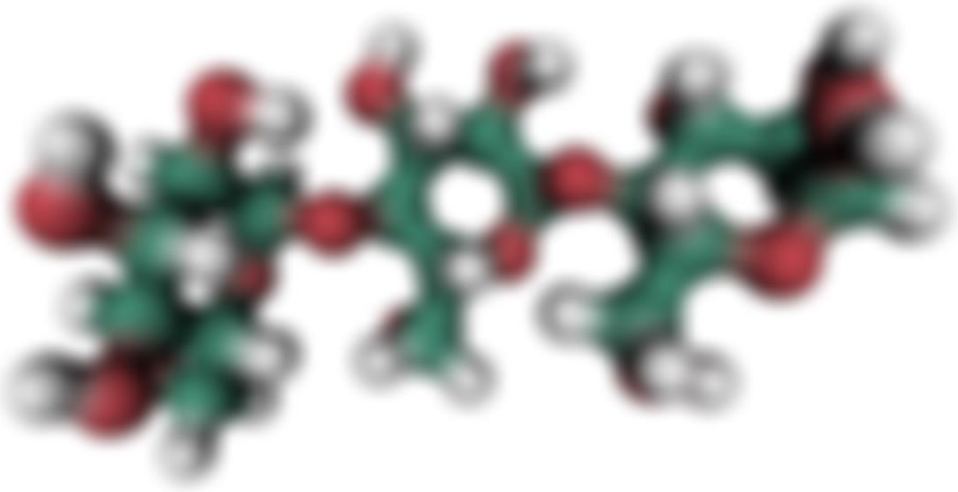
BLUR



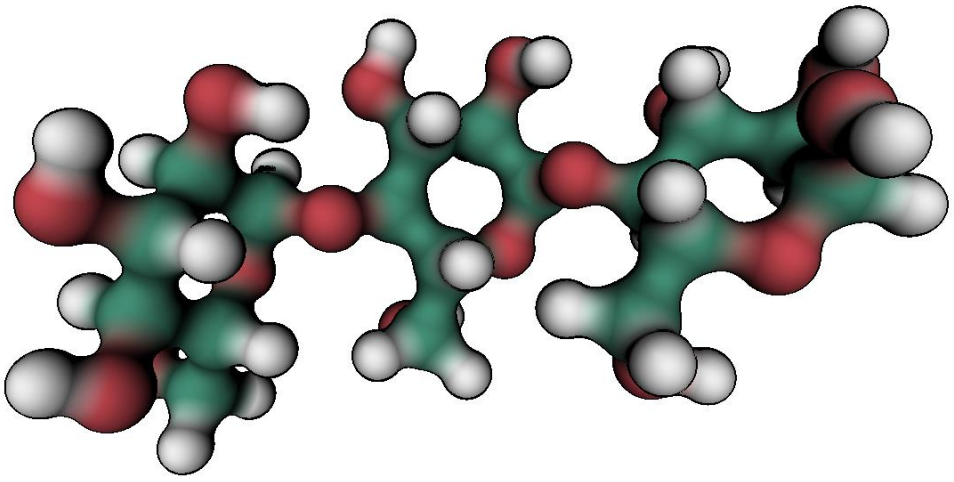
NOISE



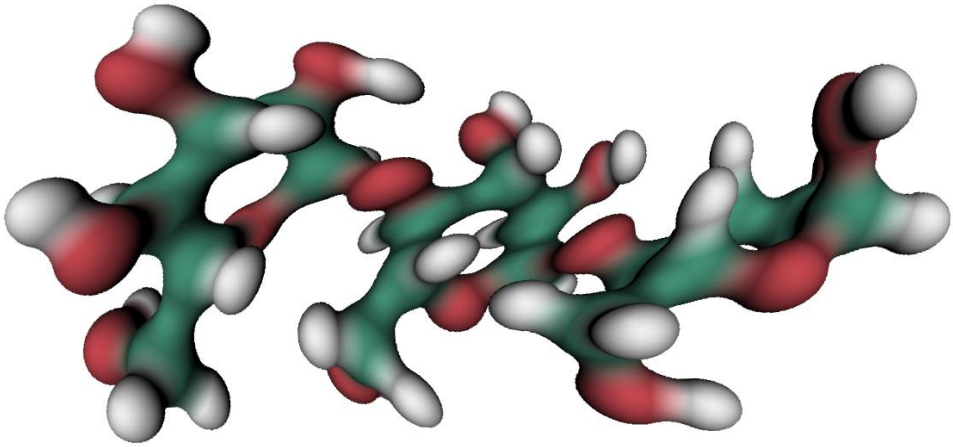
BLUR2



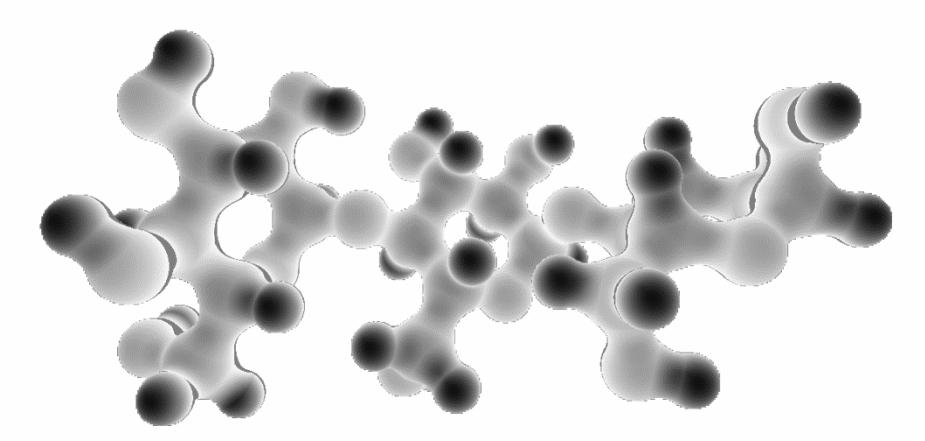
EDGE



VORTEX



GRAY



GLOW