

# Grafická reprezentace modelů molekul - VMD

# VMD

= Visual Molecular Dynamics

<http://www.ks.uiuc.edu/Research/vmd/>

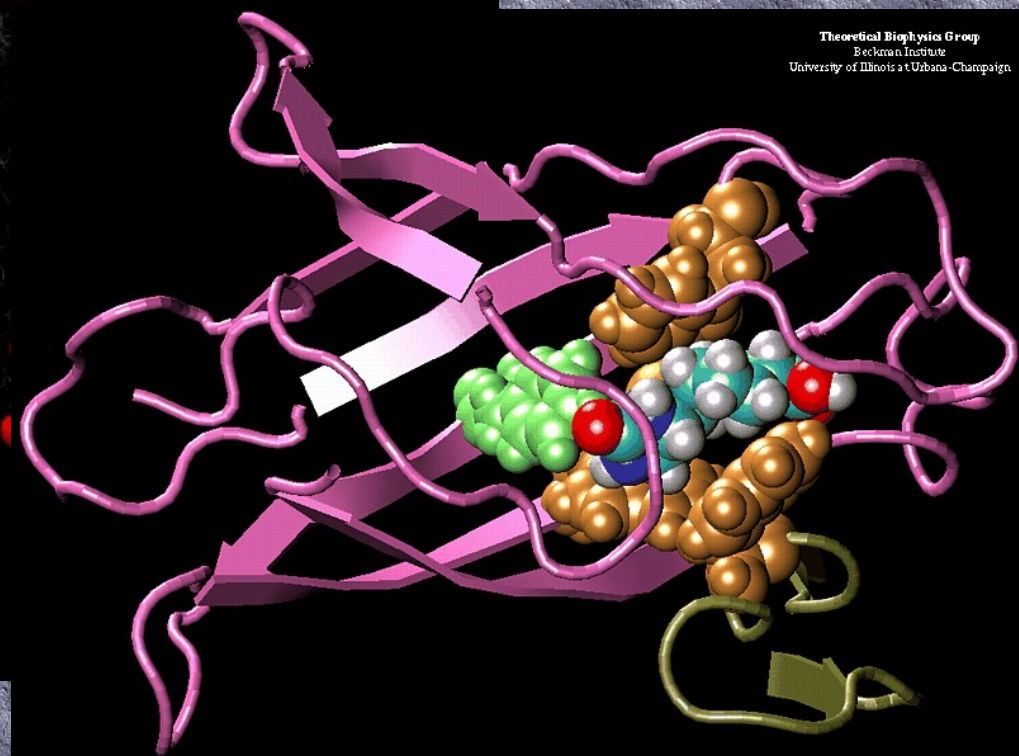
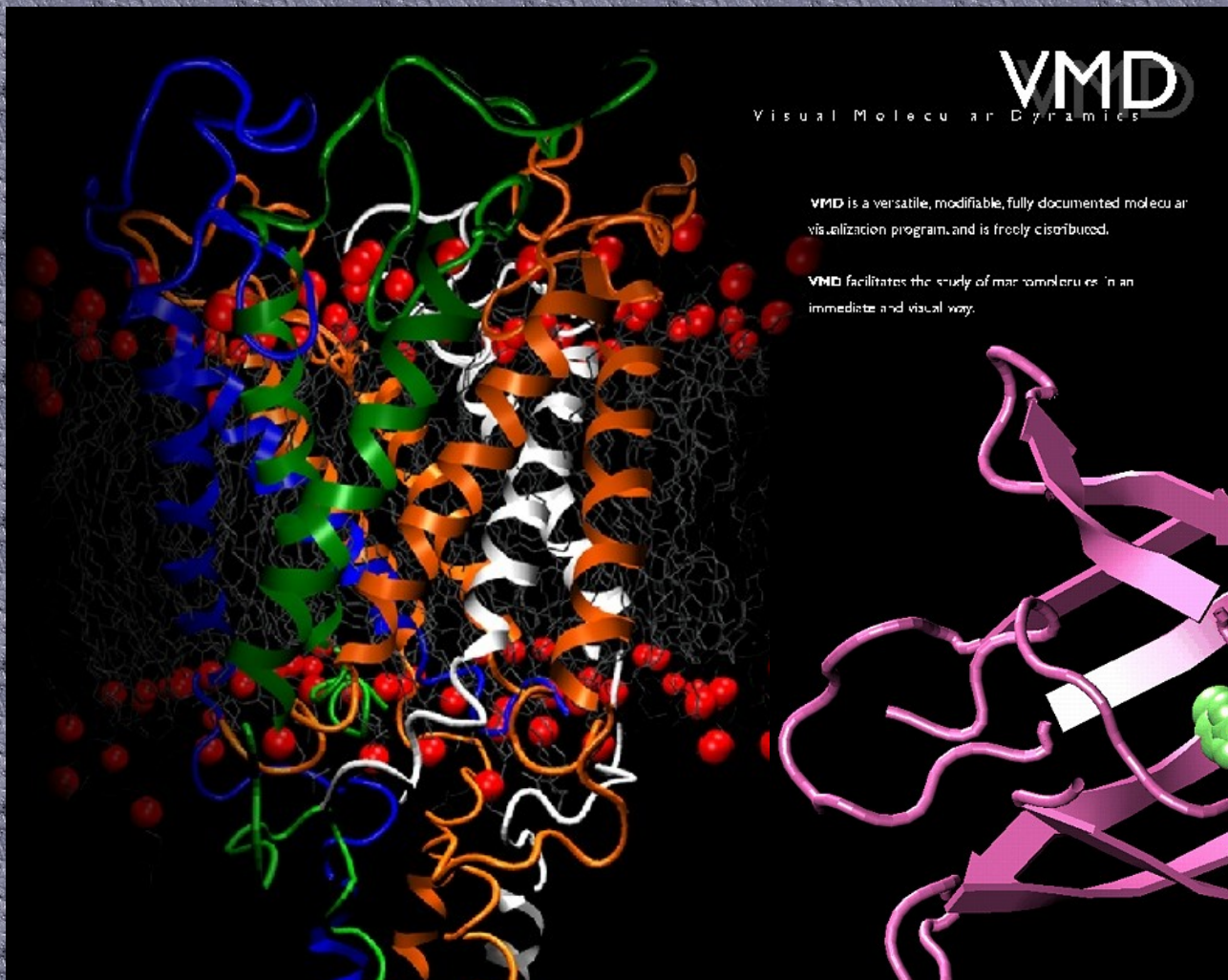
The screenshot displays the VMD software interface. The main window shows a 3D ribbon representation of a protein structure, colored in blue, green, and red. The interface includes a menu bar (Grab, File, Edit, Capture, Window, Help) and a toolbar with various controls. A 'Multiple Alignment' window is open, showing a sequence alignment for five proteins: 1LHS (Sea Turtle), 1MBA (Sea Hare), 1MBC (Sperm Whale), 1MBS (Common Seal), 1MYT (Yellowfin Tuna), and 1WLA (Horse). The alignment is displayed in a text-based format with columns for residues and markers for gaps. A 'Phylogenetic Tree' window is also visible at the bottom, showing a tree structure for the proteins.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D		1LHS (Loggerhead Sea)	2731	1	0
1		A	D	F	1MBA (Sea Hare)	2552	1	0
2		A	D		1MBC (Sperm Whale)	2943	1	0
3		A	D		1MBS (Common Seal)	2945	1	0
4		A	D		1MYT (Yellowfin Tuna)	2539	1	0
5		A	D		1WLA (Horse)	2706	1	0

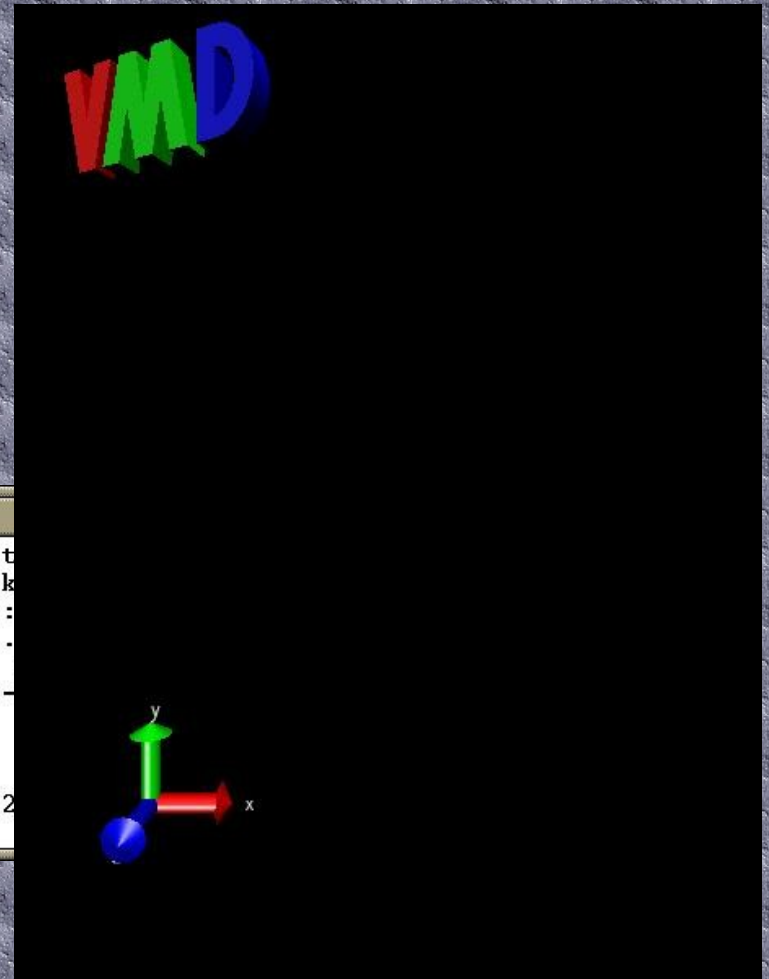
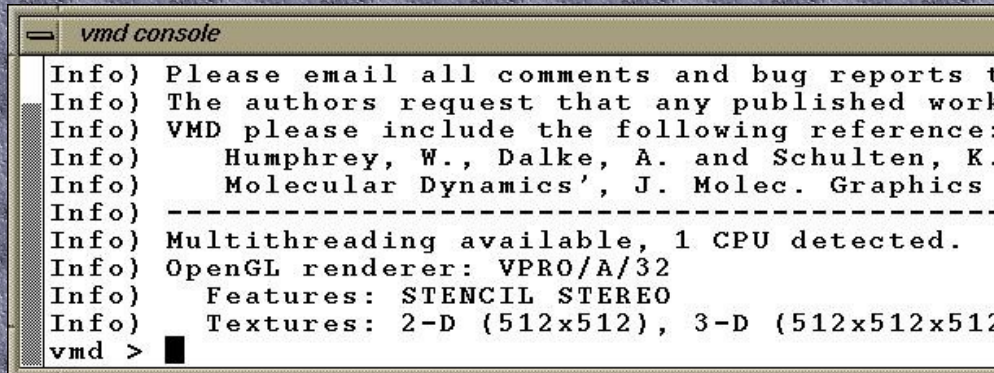
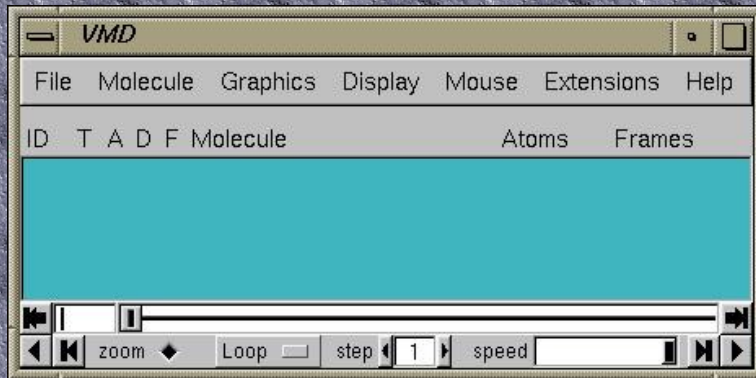
```
{1LHS (Sea Turtle)}  XPETQERFAKFNLTIDALKSSEEVKKXGTVL TALGRILKQK--NN-XEQELK
{1MBA (Sea Hare)}   IFDSANFFADDFGKS-VADIKASPKLRDVSSRIFTRLNEFVNNAANAGKMSAMLS
{1MBC (Sperm Whale)} XPETLEKFDKFKXKTEAEMKASEDLKXGTVL TALGAILKKK--GX-XEAEK
{1MBS (Common Seal)} XPETLEKFDKFKXKSEDDMRSEDLRXXGTVL TALGGILKKK--GX-XEAEK
{1MYT (Yellowfin Tuna)} XPETQKLPFKFAGIA-QADIAGNAAISXGATV LKLGELKAK--GS-XAAILK
{1WLA (Horse)}      XPETLEKFDKFKXKTEAEMKASEDLKXGTVL TALGGILKKK--GX-XEAEK
                    40 + 50 + 60 + 70 + 80 + 90
```

Platformy: LINUX, IRIX (SGI), Windows, MAC ...

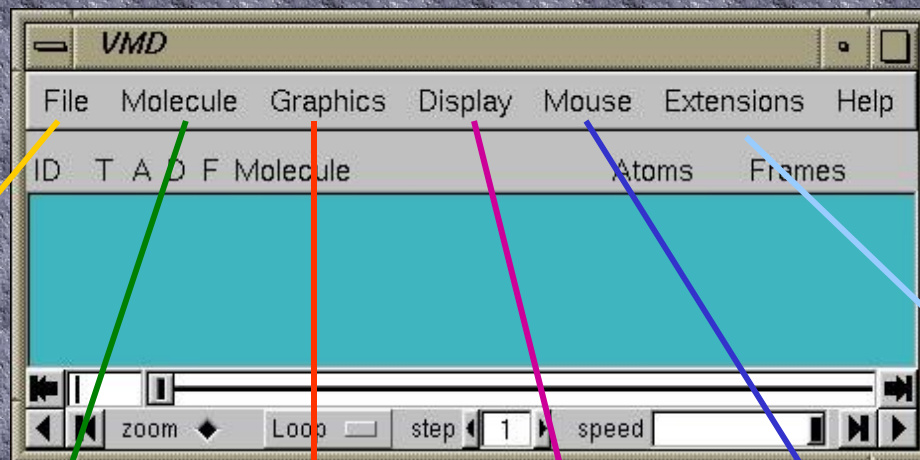
# VMD



# Náhled programu



# Menu a příkazy



- Load Molecule...
- Load State...
- Save Trajectory...
- Save State...
- Render...
- Quit

- Make Top
- Toggle Active
- Toggle Displayed
- Toggle Fixed
- Rename
- Cancel File I/O
- Delete Timesteps
- Delete Molecule

- Representations...
- Colors...
- Materials...
- Labels...
- Tools...
- Simulation...

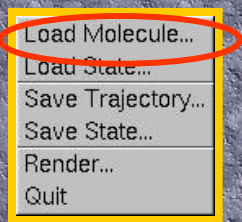
- Reset View
- Stop Rotation
- Perspective
- Orthographic
- Antialiasing
- Depth Cueing
- Culling
- FPS Indicator
- Light 0
- Light 1
- Light 2
- Light 3
- Axes ▶▶▶
- Stage ▶▶▶
- Stereo ▶▶▶
- Settings...

- Rotate Mode r
- Translate Mode t
- Scale Mode s
- Pick ▶▶▶
- Move ▶▶▶
- Force ▶▶▶
- Move Light ▶▶▶
- Add/Remove Bonds

- sequence
- ramaplot
- AutoIMD
- aligntool
- contactmap
- timeline
- vmdmovie
- solvate

# Načtení molekuly

dimethylfosfát



# Grafická reprezentace

Representations...

Colors...

Materials...

Labels...

Tools...

Simulation...

**Graphical Representations**

Selected Molecule  
0: dmp.pdb

Create Rep Delete Rep

Style	Color	Selection
Lines	Name	all

Selected Atoms  
all

Draw style | Selections | Smoothing |

Coloring Method: Name  
Material: Transparent

Drawing Method: Lines

Thickness: 1

Update Selection Every Frame  Apply Changes Automatically

Lines

Bonds

DynamicBonds

HBonds

Points

VDW

CPK

Licorice

Trace

Tube

Ribbons

NewRibbons

Cartoon

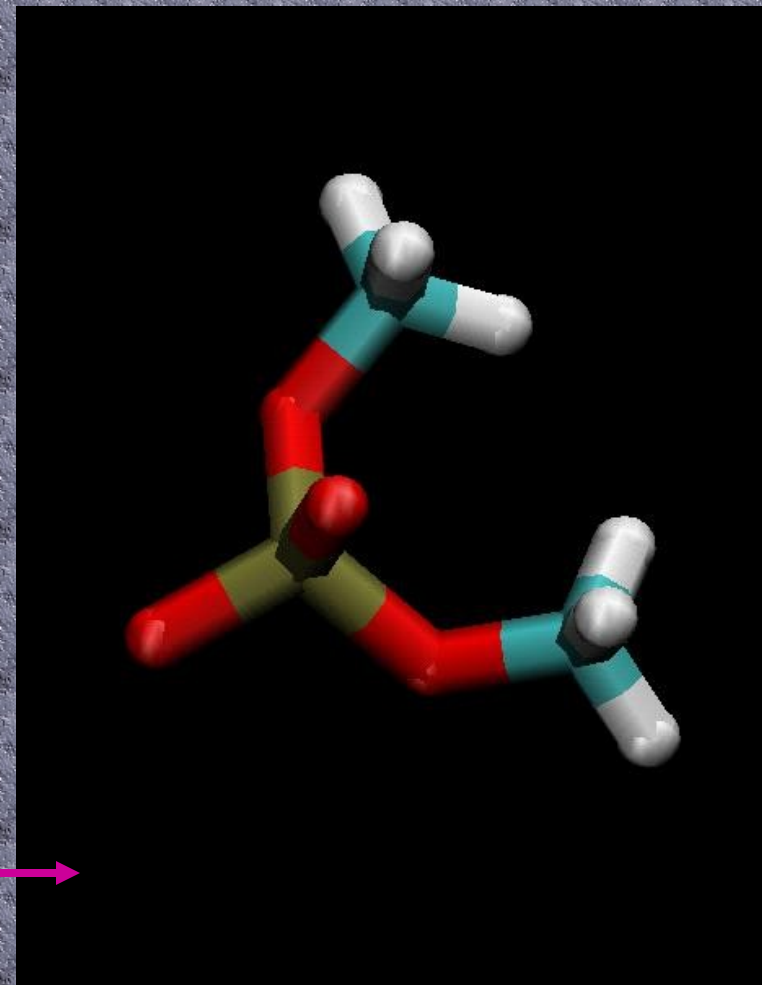
MSMS

Surf

VolumeSlice

Isosurface

Dotted



# Další modely...

**Graphical Representations**

Selected Molecule  
0: dmp.pdb

Create Rep Delete Rep

Style	Color	Selection
VDW	Name	all
CPK	Name	all

Selected Atoms  
all

Draw style \ Selections \ Smoothing \

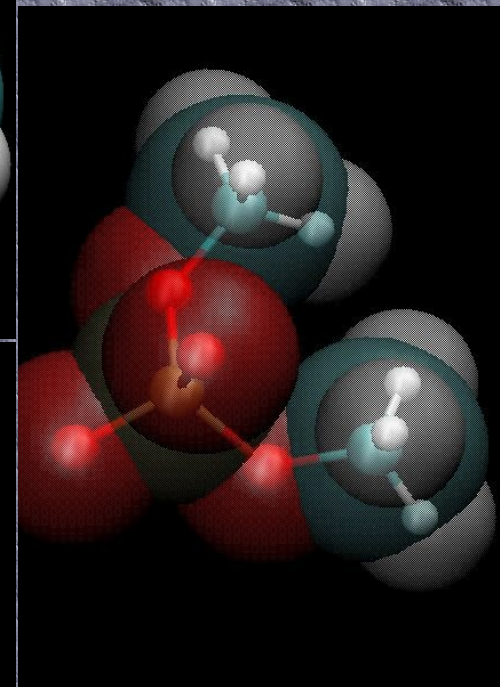
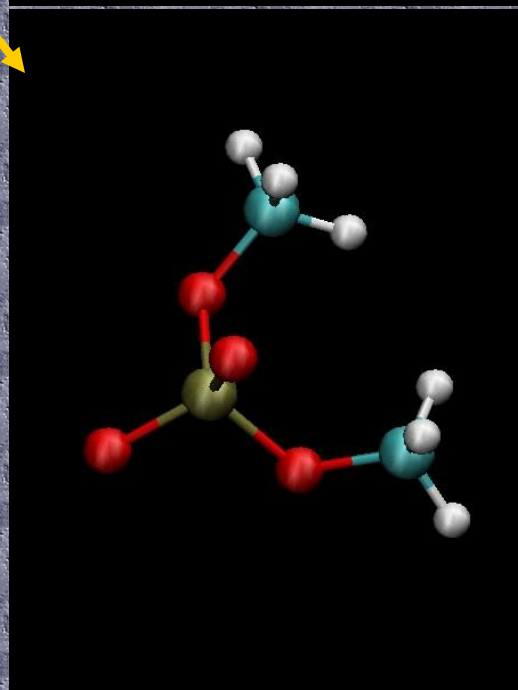
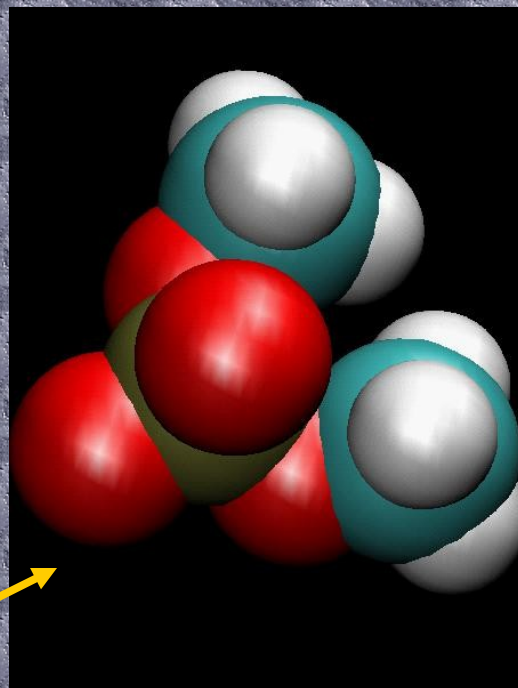
Coloring Method Material  
Name Transparent

Drawing Method  
VDW Default

Sphere Radius 1.0  
Sphere Resolution 20

Update Selection Every Frame Apply Changes Automatically Apply

- Lines
- Bonds
- DynamicBonds
- HBonds
- Points
- VDW
- CPK
- Licorice
- Trace
- Tube
- Ribbons
- NewRibbons
- Cartoon
- MSMS
- Surf
- VolumeSlice
- Isosurface
- Dotted

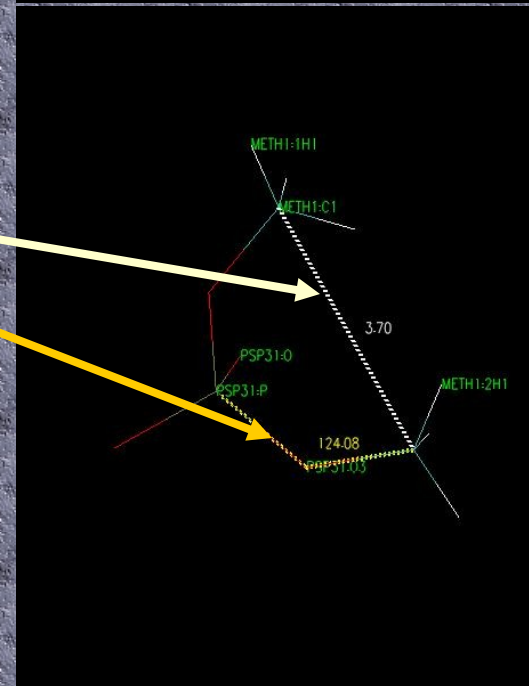
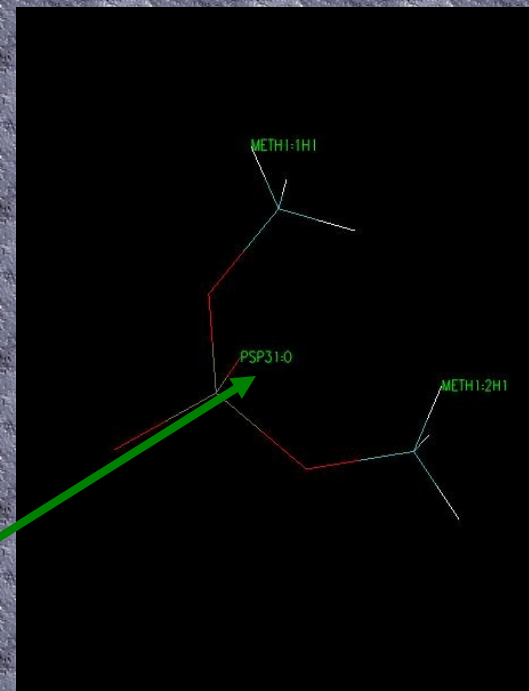




# Popisy atomů, měření geometrie

- ◇ Rotate Mode r
- ◆ Translate Mode t
- ◇ Scale Mode s
- Pick
- Move
- Force
- Move Light
- ◇ Add/Remove Bonds

- ◇ Center c
- ◇ Atoms 1
- ◇ Bonds 2
- ◇ Angles 3
- ◇ Dihedrals 4



# Změna barev

Graphical Representations

Selected Molecule  
0: dmp.pdb

Create Rep Delete Rep

Style	Color	Selection
VDW	ColorID 9	all
CPK	ColorID 0	all

Selected Atoms  
all

Draw style | Selections | Smoothing

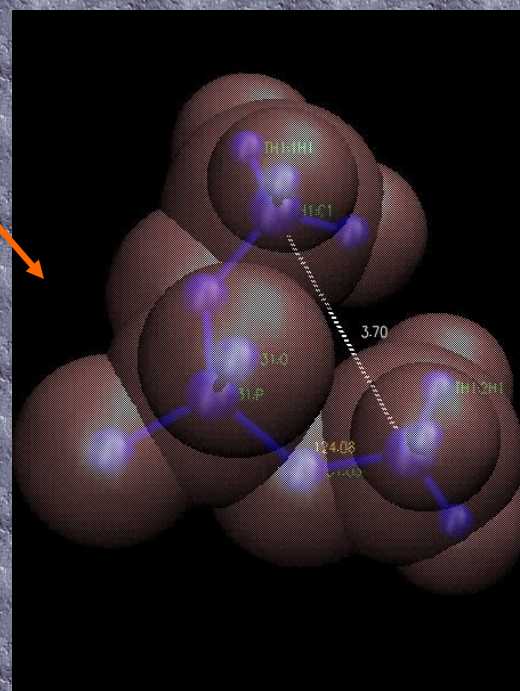
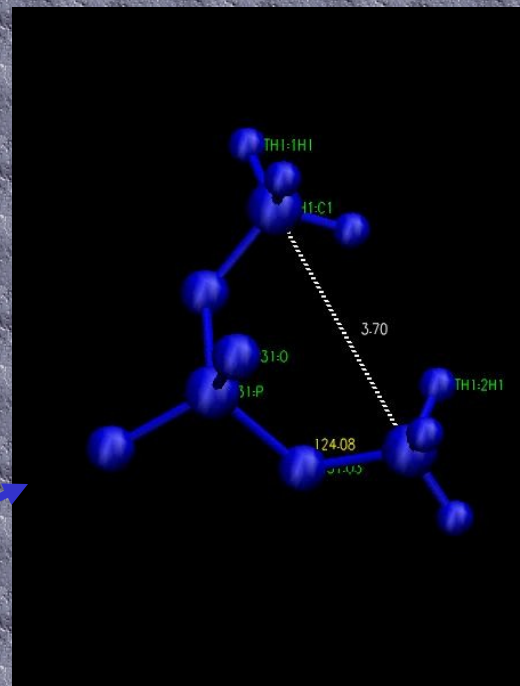
Coloring Method: ColorID  Material: Transparent

Drawing Method: VDW  Default

Sphere Radius:

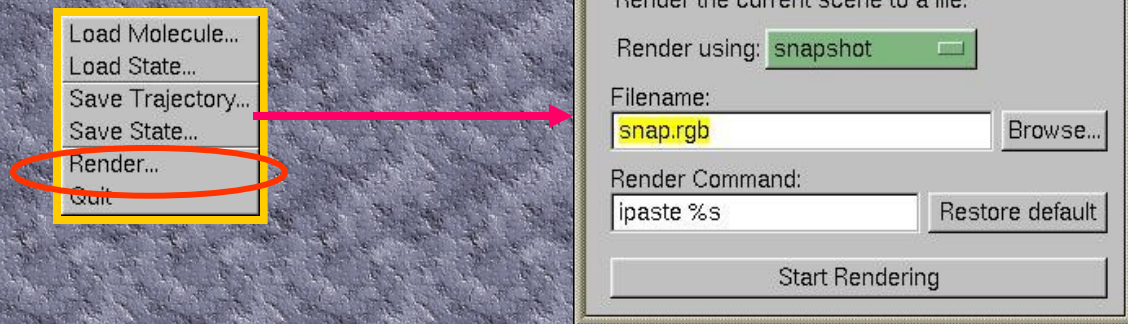
Sphere Resolution:

Update Selection Every Frame  Apply Changes Automatically

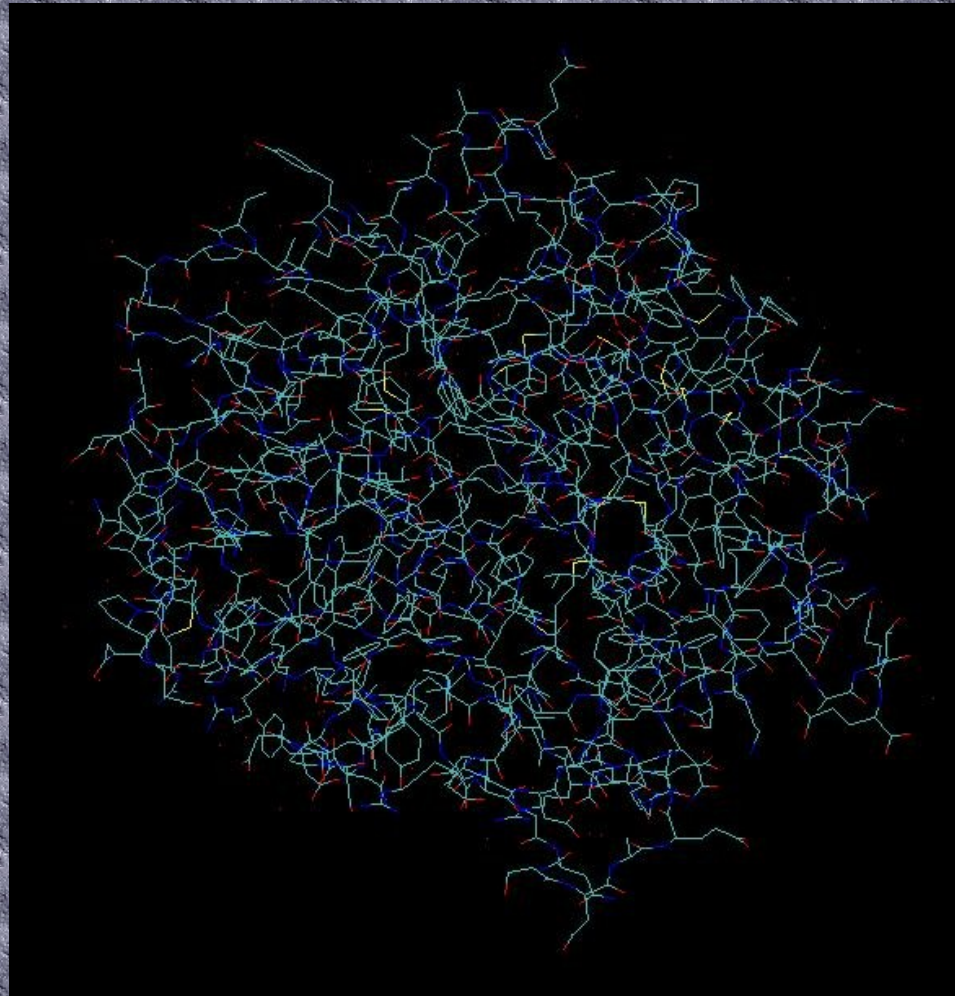


- Name
- Type
- ResName
- ResType
- ResID
- Chain
- SegName
- Molecule
- Structure
- ColorID**
- Beta
- Occupancy
- Mass
- Charge
- Pos
- Index
- Backbone
- Throb

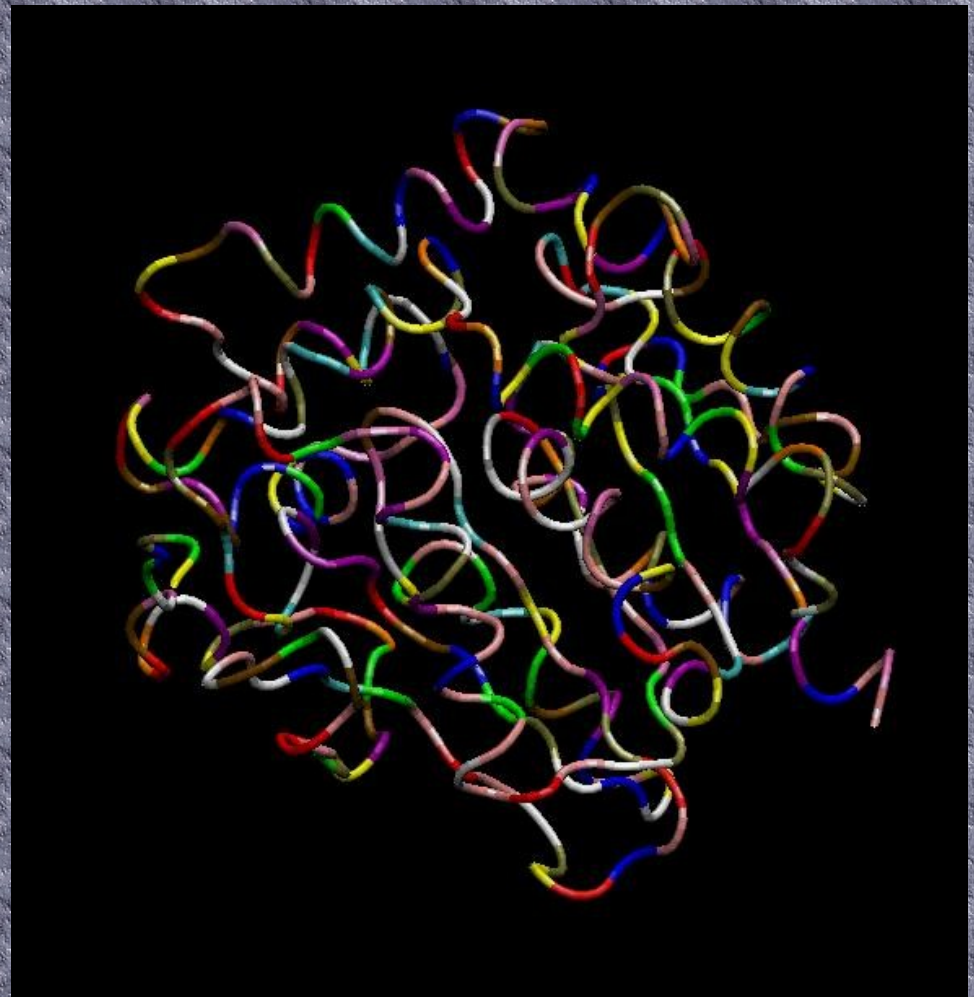
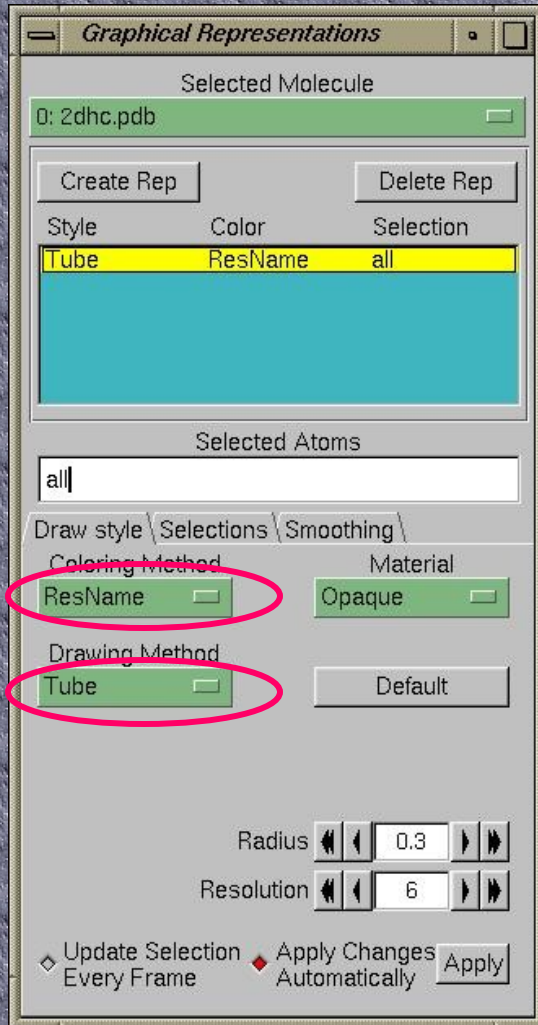
# Export (uložení) obrázku



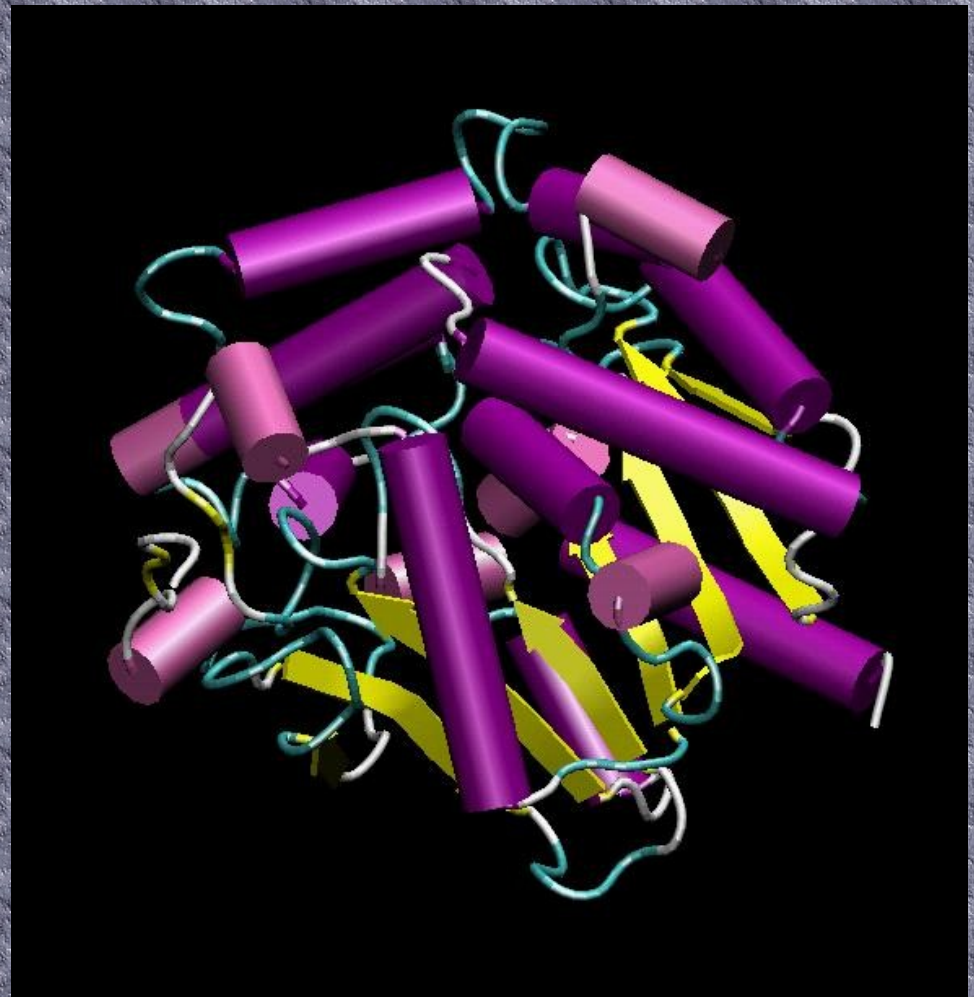
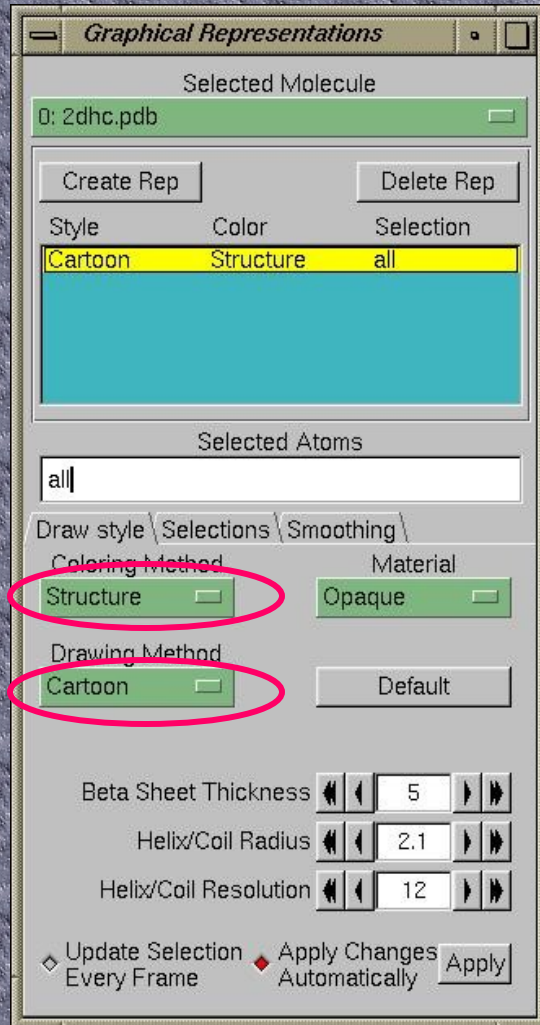
# Zobrazení proteinu



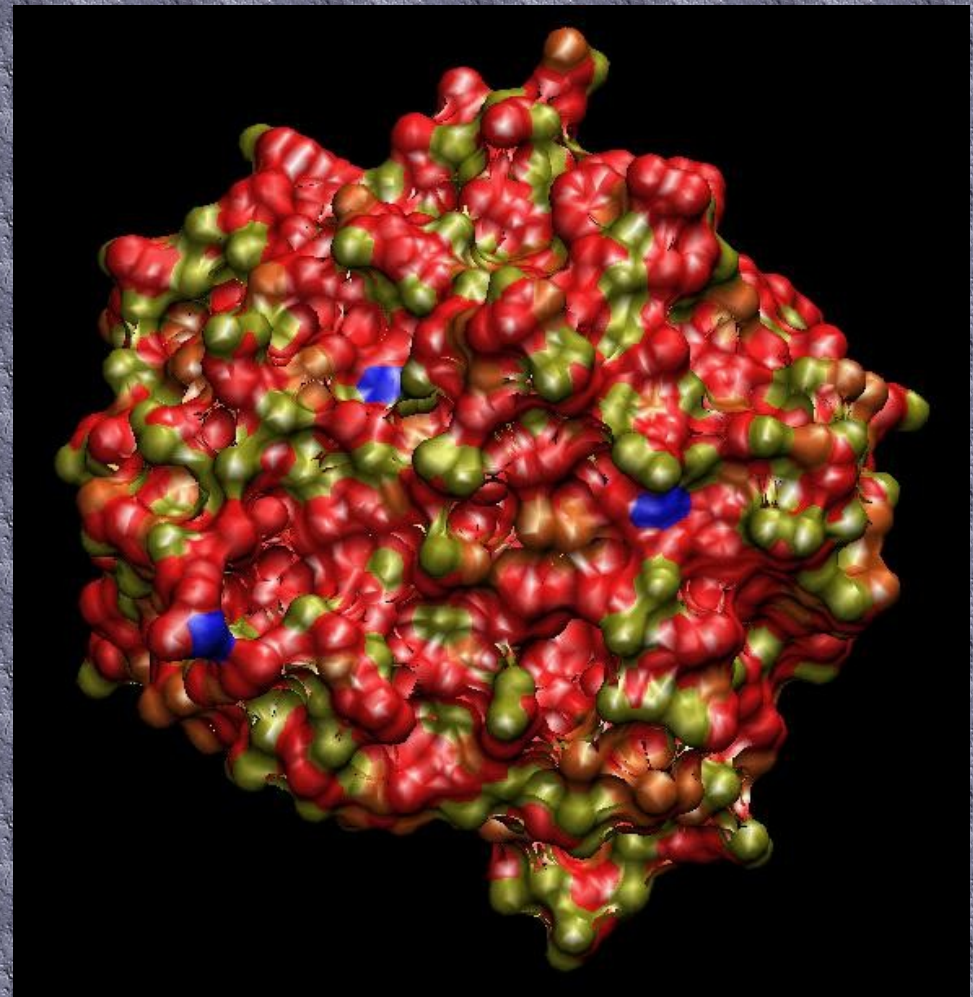
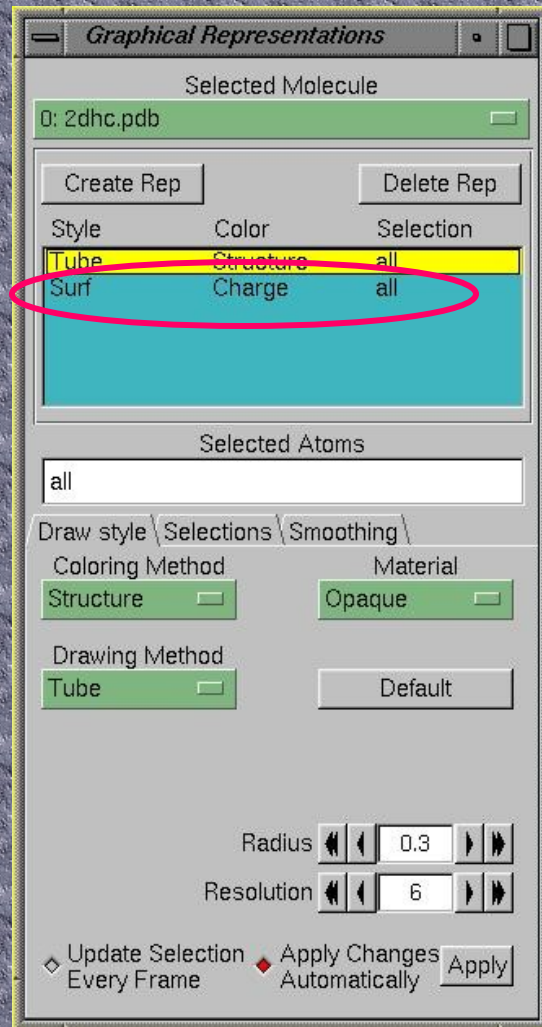
# Páteř proteinu



# Sekundární struktury



# Povrch proteinu



# Povrch proteinu

**Graphical Representations**

Selected Molecule  
0: 2dhc.pdb

Create Rep      Delete Rep

Style	Color	Selection
Tube	Structure	all
Surf	Charge	all

Selected Atoms  
all

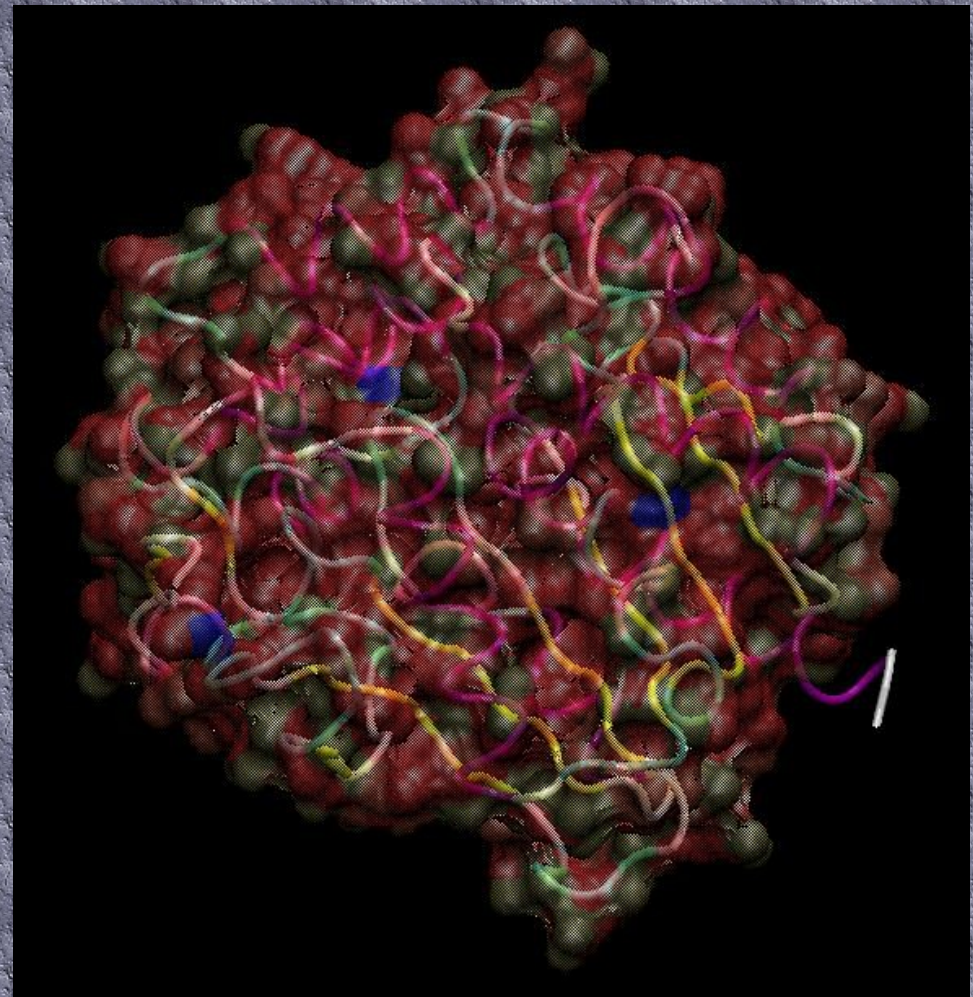
Draw style | Selections | Smoothing |

Coloring Method      Material  
Structure      Opaque

Drawing Method  
Tube      Default

Radius      0.3  
Resolution      6

Update Selection Every Frame       Apply Changes Automatically      Apply





# Povrchy (surfaces)

## vdW povrch

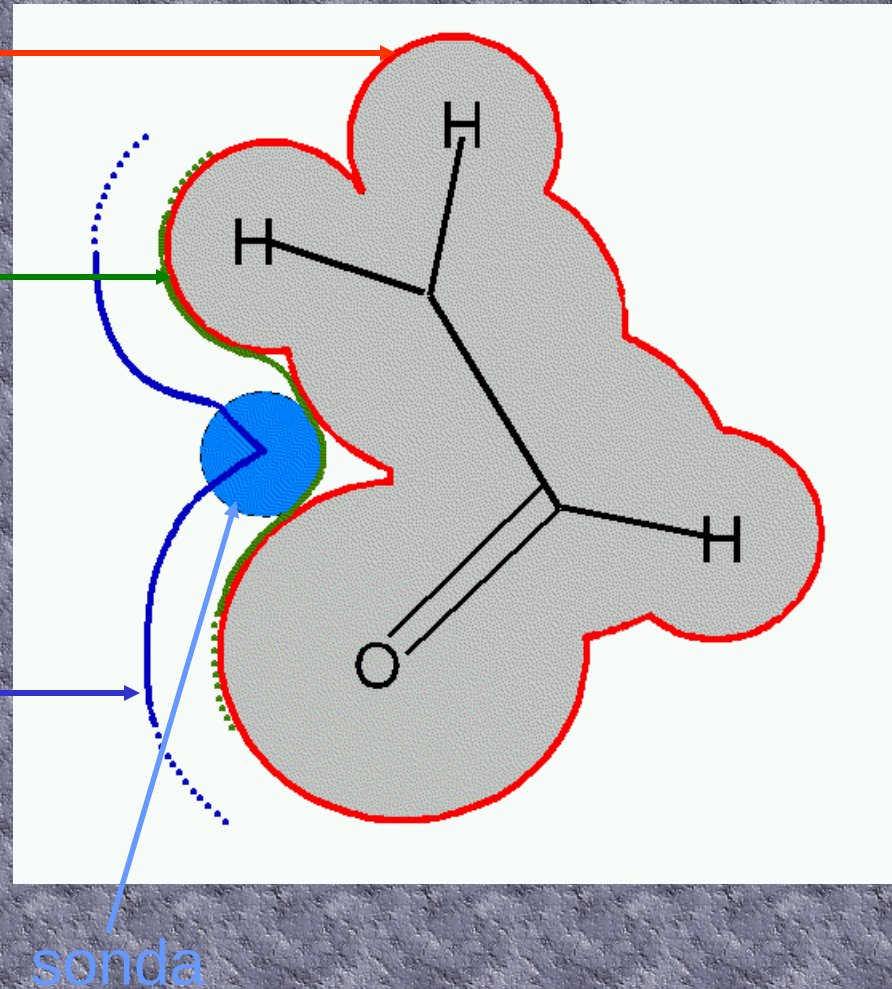
obal založený na vdW poloměrech atomů

## Connolyho povrch

povrch molekuly, který je přístupný sondě o urč. poloměru

Povrch přístupný solventu  
= Solvent Accessible  
Surface Area (SASA)

obal molekuly, který je přístupný středu sondy o urč. poloměru

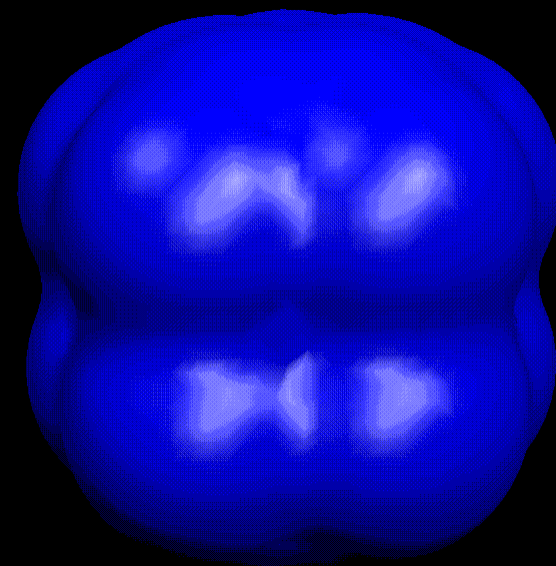
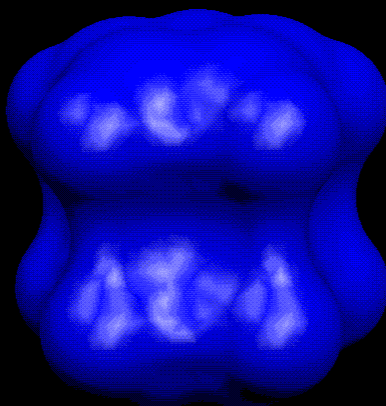
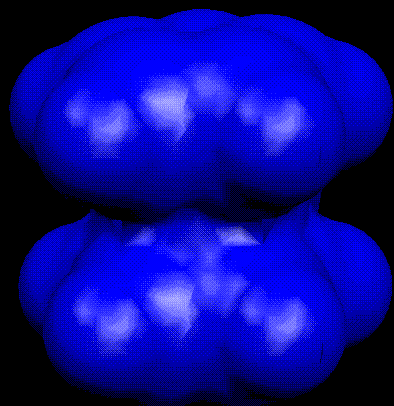


# Srovnání povrchů

vdW

Connolly

SASA



# Modely vybraných částí...

**Graphical Representations**

Selected Molecule  
0: 2dhc.pdb

Create Rep Delete Rep

Style	Color	Selection
Lines	Name	all
VDW	Name	resid 15
VDW	ColorID 3	rename VAL and name C
CPK	ColorID 7	within 5 of resid 58

Selected Atoms  
within 5 of resid 58

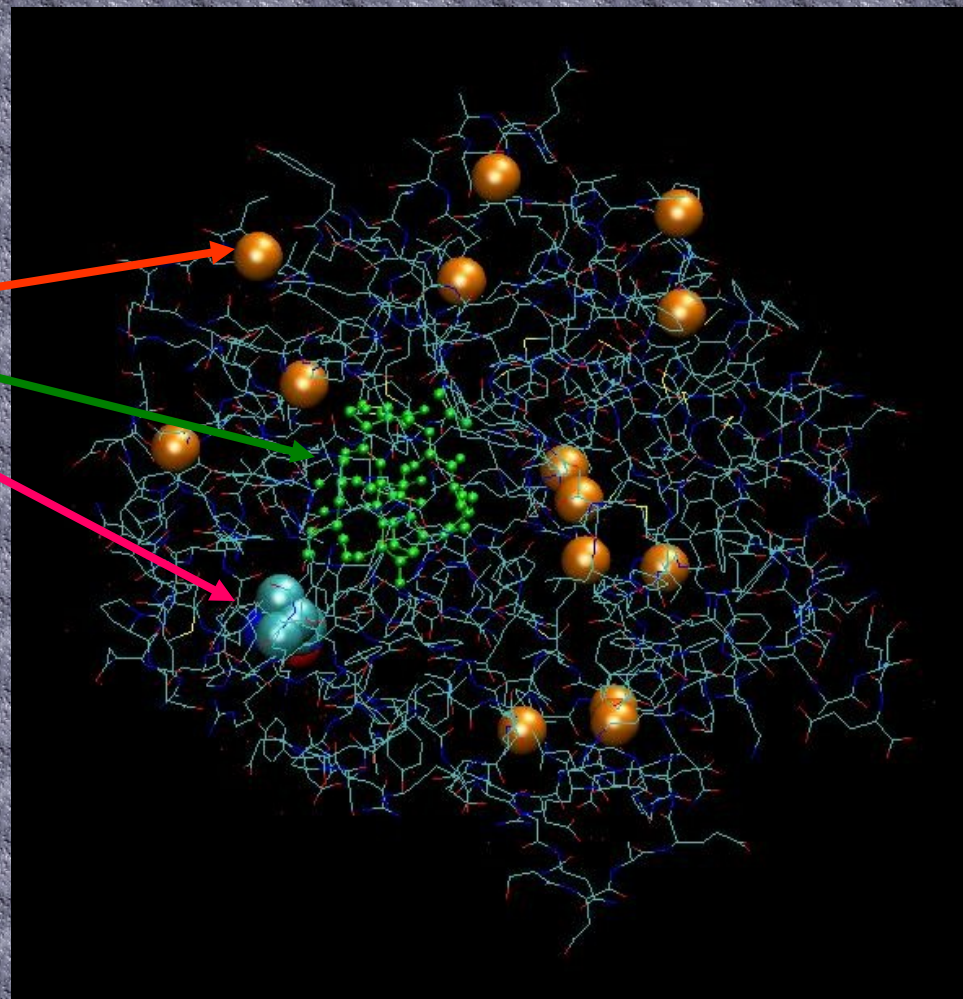
Draw style \ Selections \ Smoothing \

Coloring Method Material  
ColorID 7 Opaque

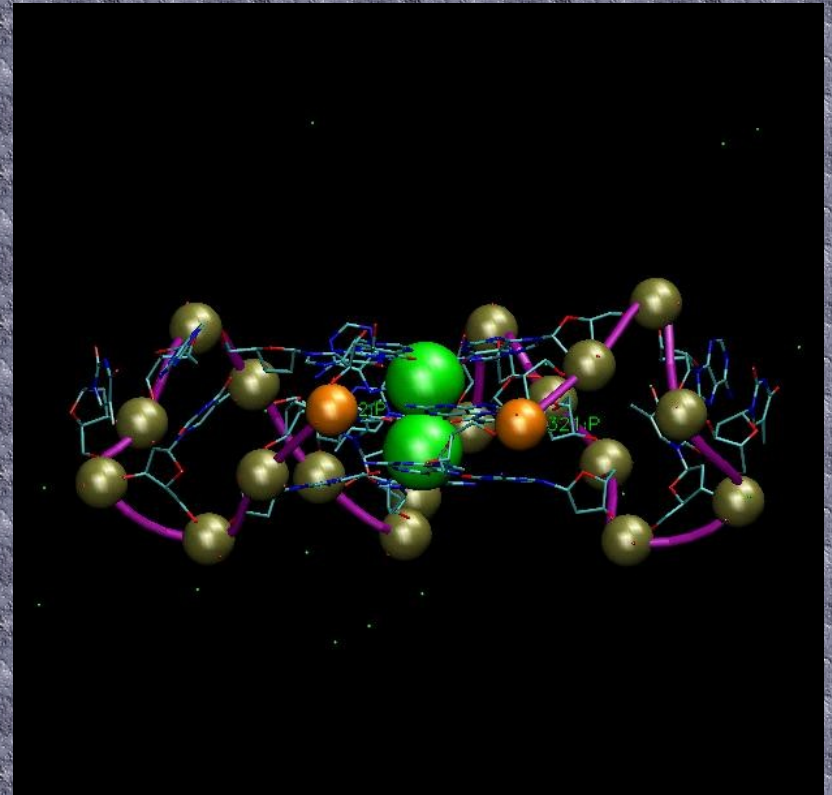
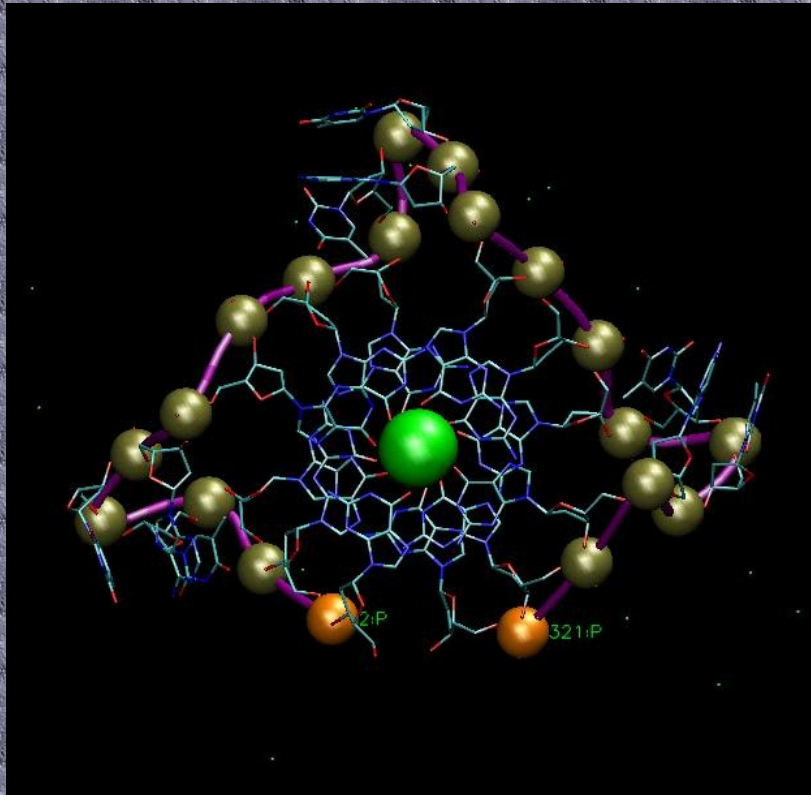
Drawing Method  
CPK Default

Sphere Radius 1.0  
Sphere Resolution 8  
Bond Radius 0.3  
Bond Resolution 6

Update Selection Every Frame Apply Changes Automatically Apply



# Human telomere...



Cvičení...