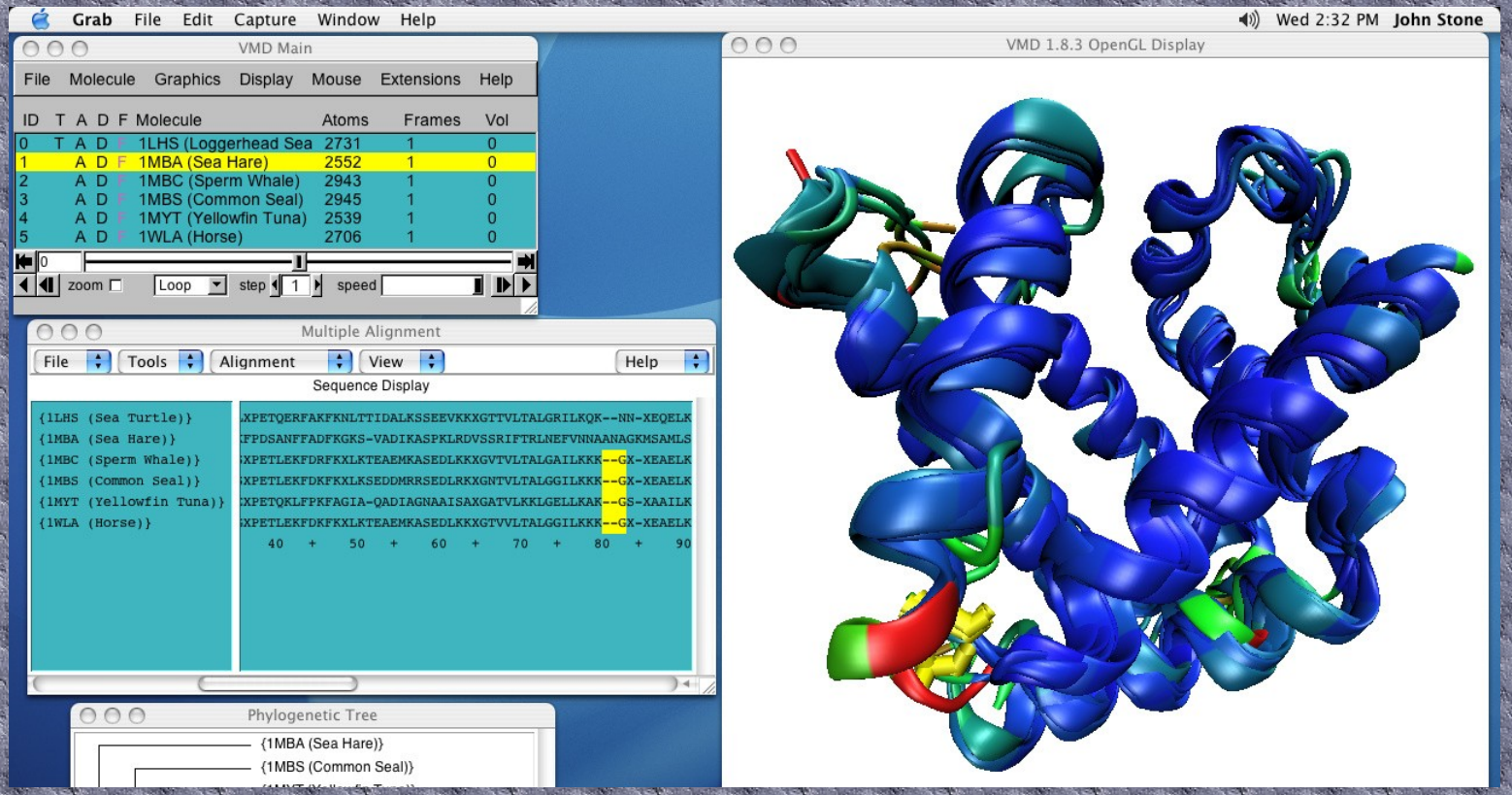
Grafická reprezentace modelů molekul - VMD

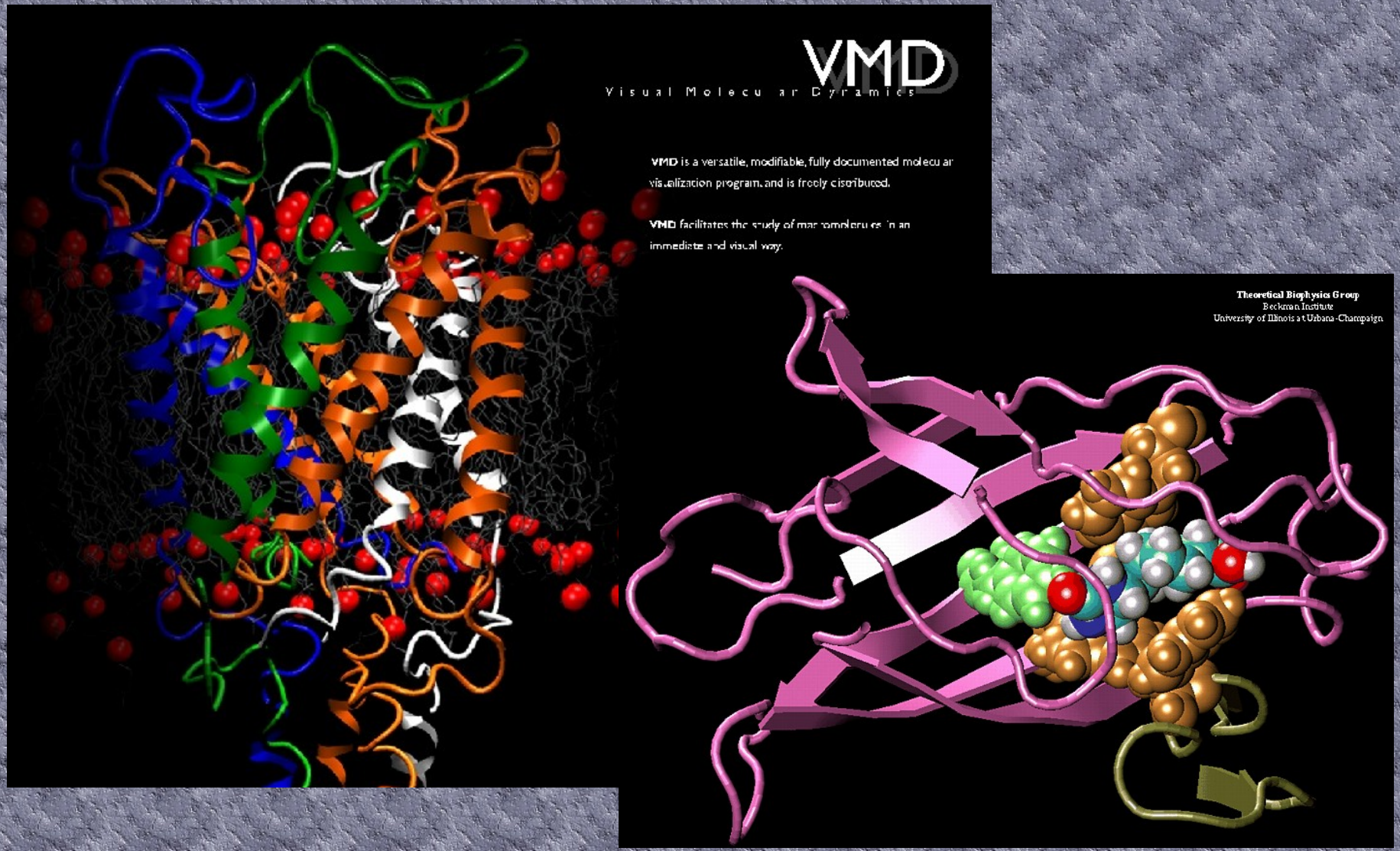
VMD
= Visual Molecular Dynamics

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

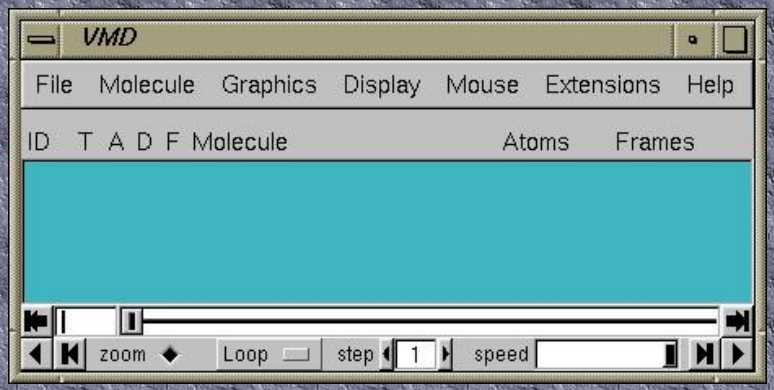


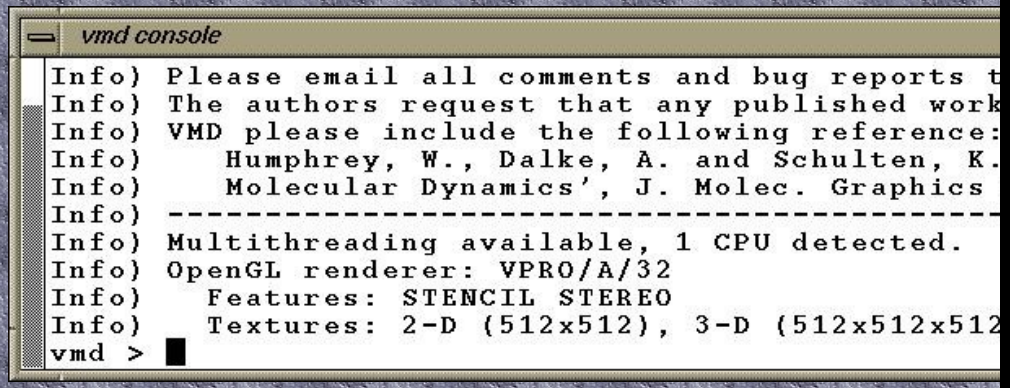
Platformy: LINUX, IRIX (SGI), Windows, MAC ...

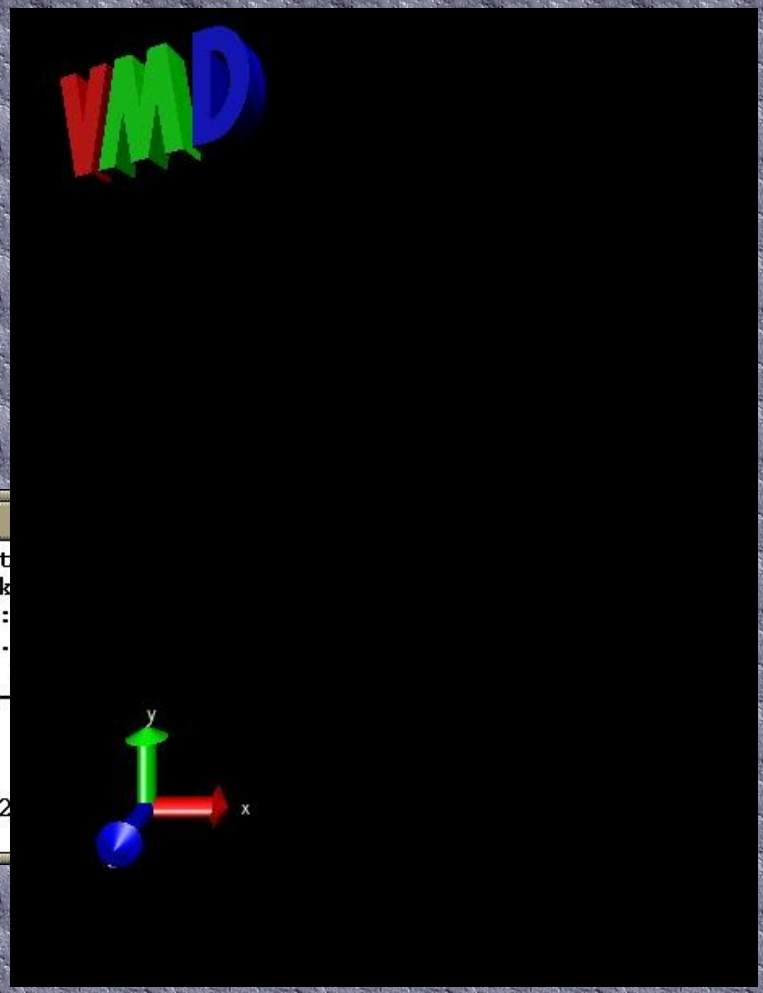
VMD


VMD
Visual Molecular Dynamics
VMD is a versatile, modifiable, fully documented molecular visualization program, and is freely distributed.
VMD facilitates the study of macromolecules in an immediate and visual way.
Theoretical Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign

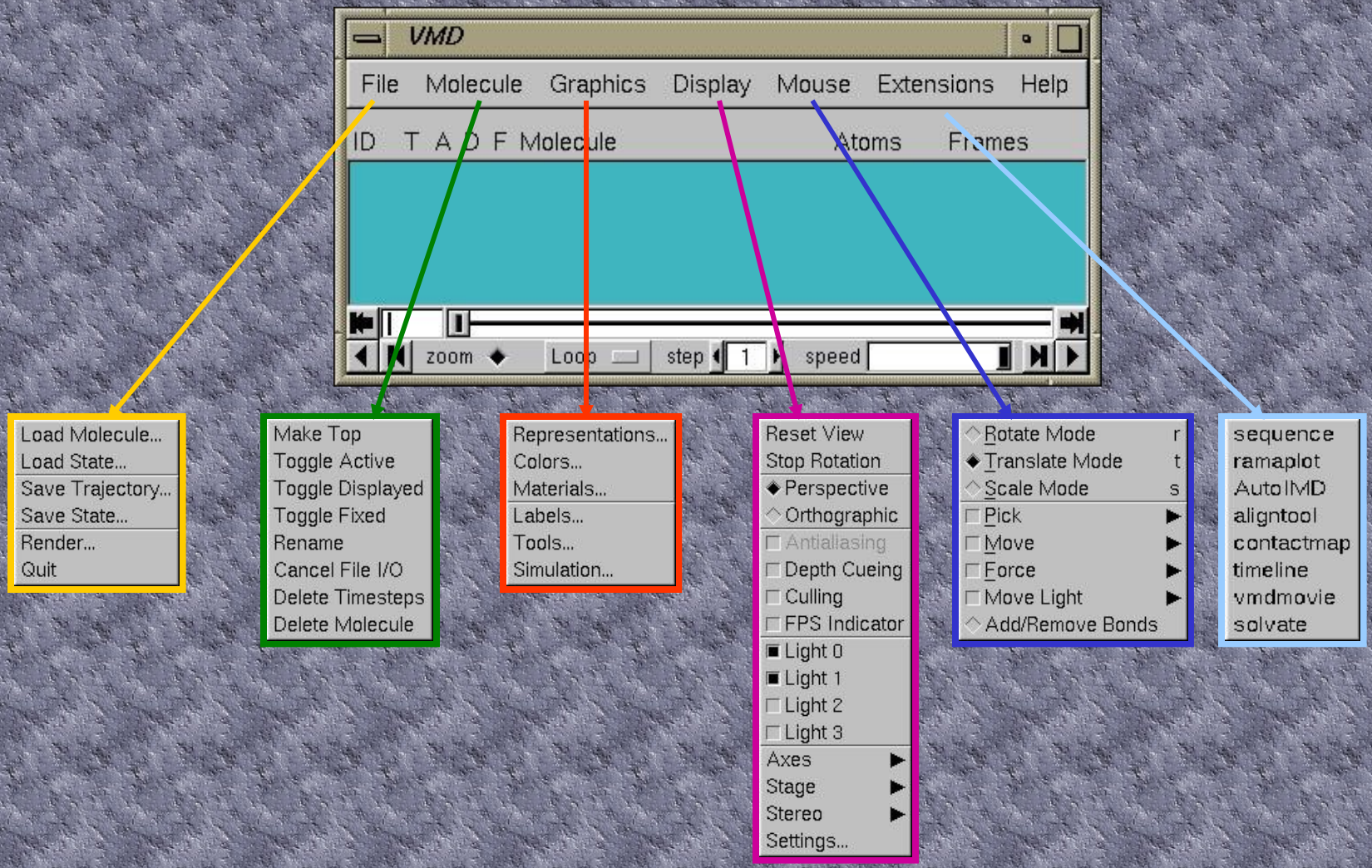
Náhled programu





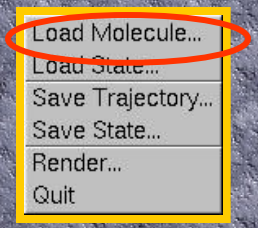


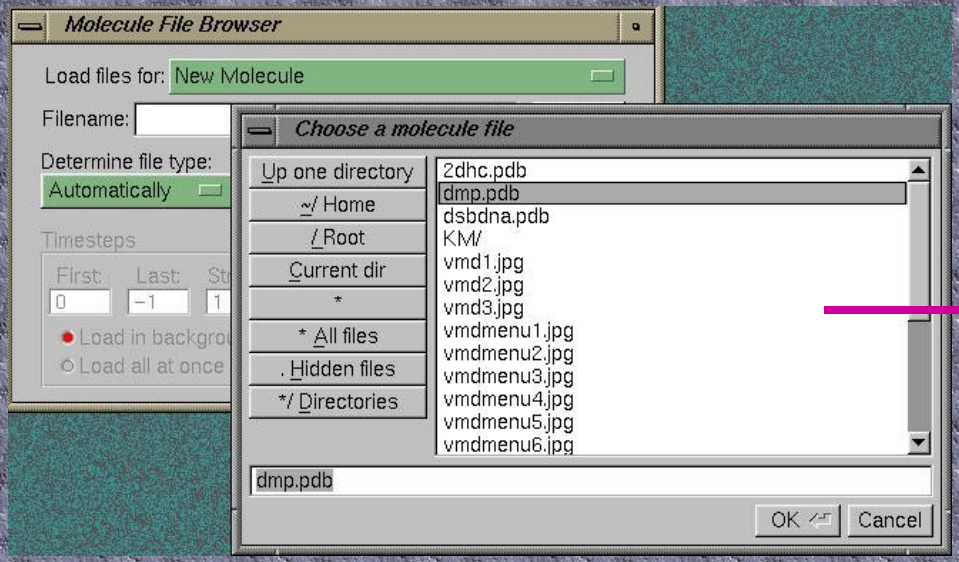
Menu a příkazy



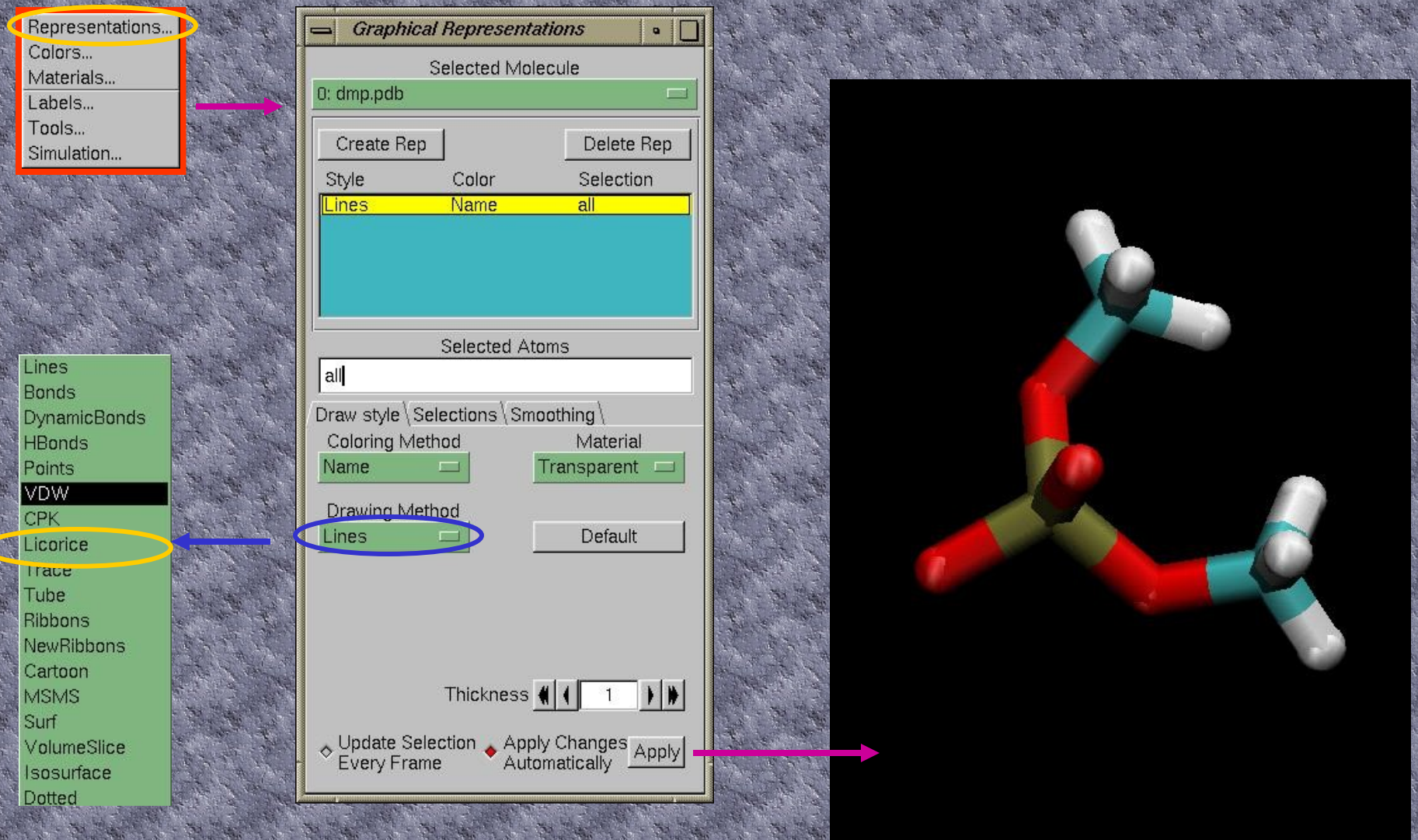
Načtení molekuly

dimethylfosfát

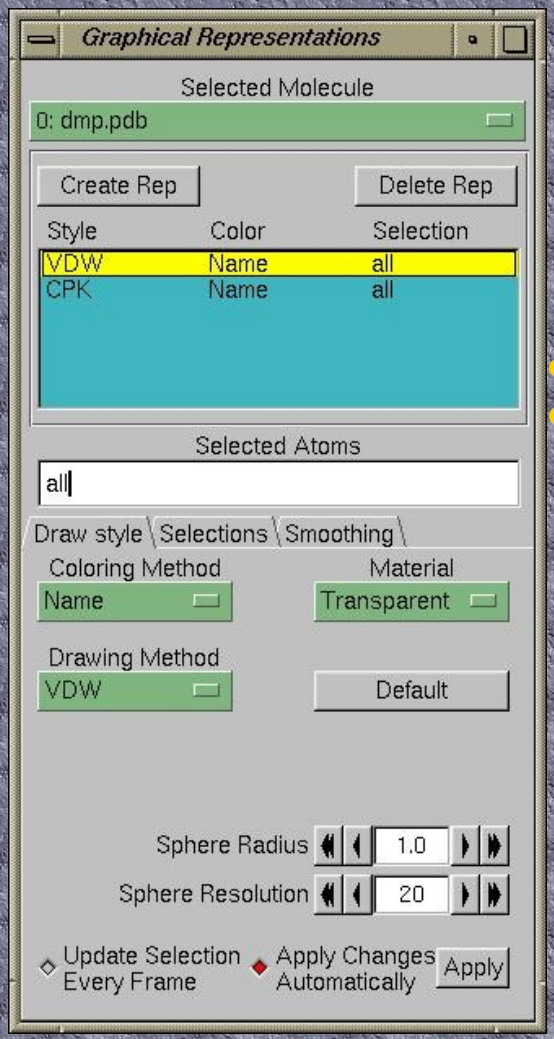


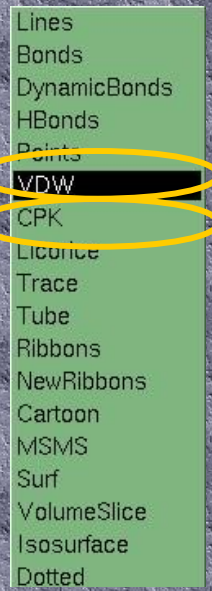


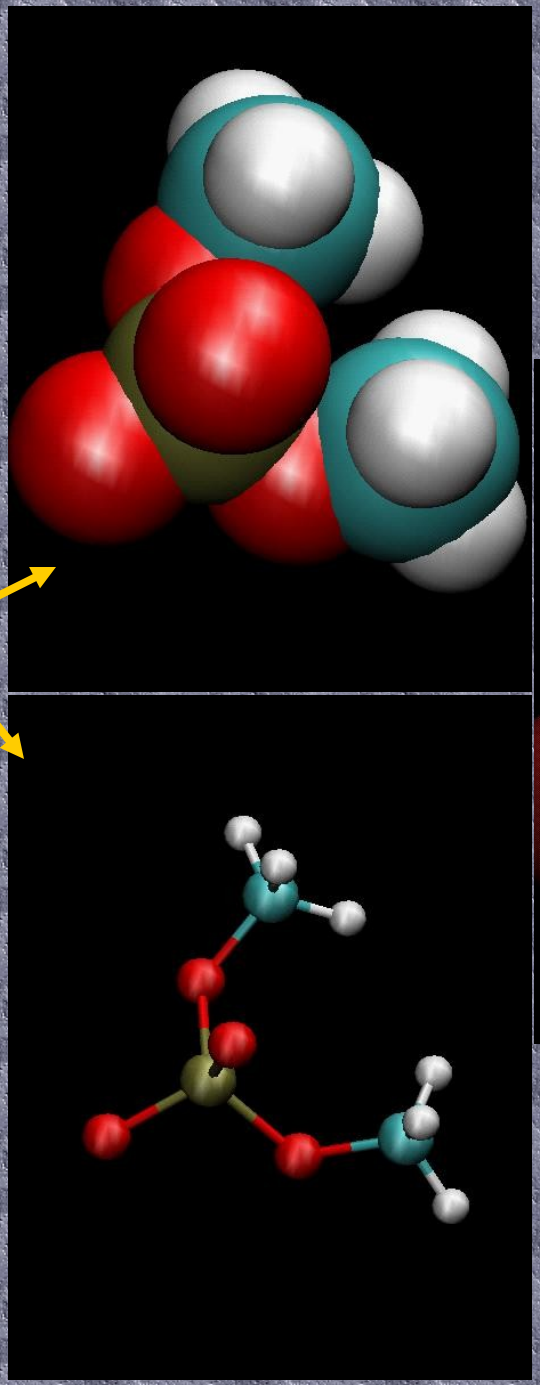
Grafická reprezentace

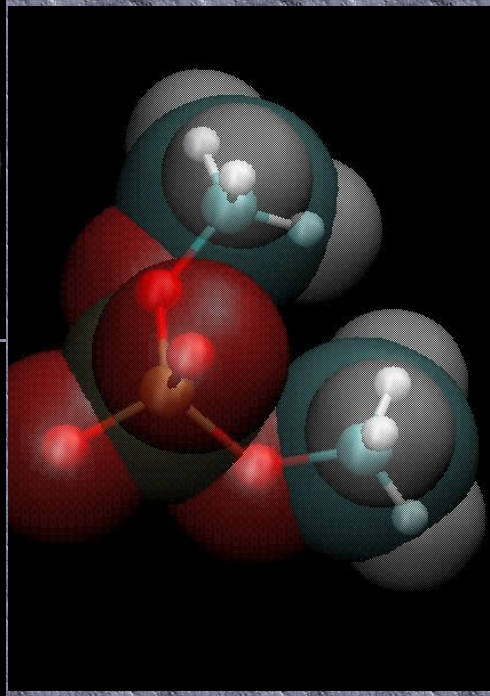


Další modely…

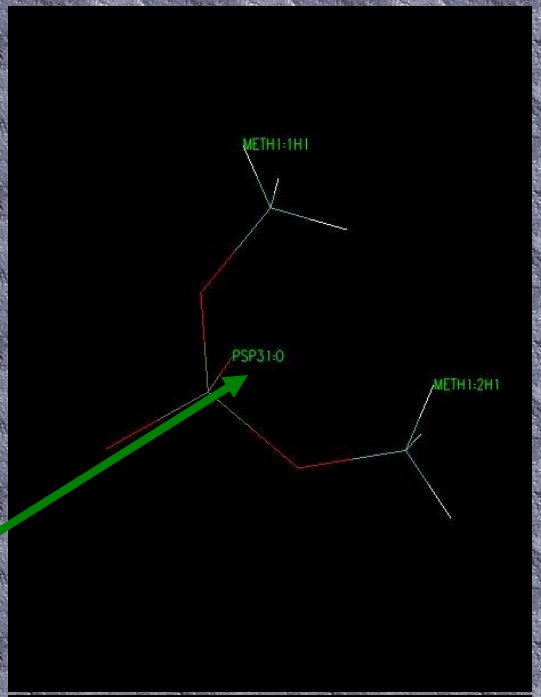


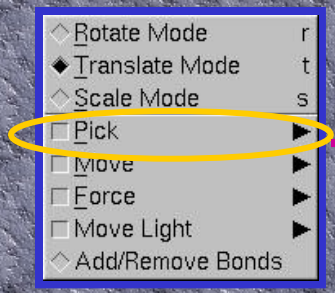


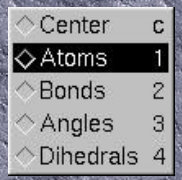


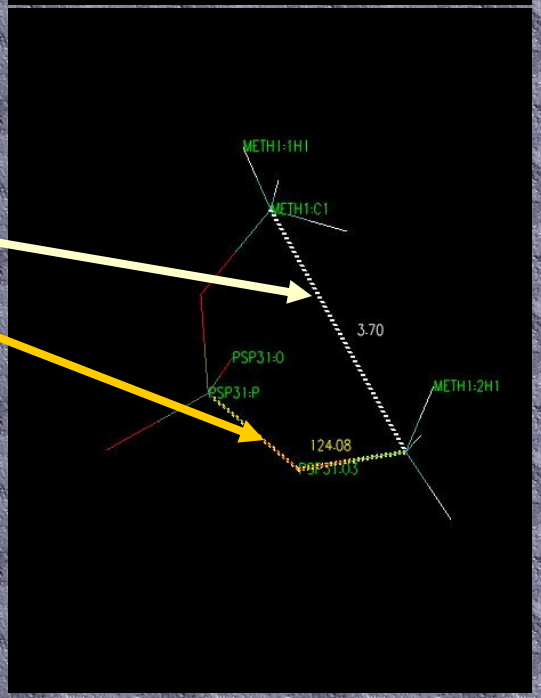


Popisy atomů, měření geometrie

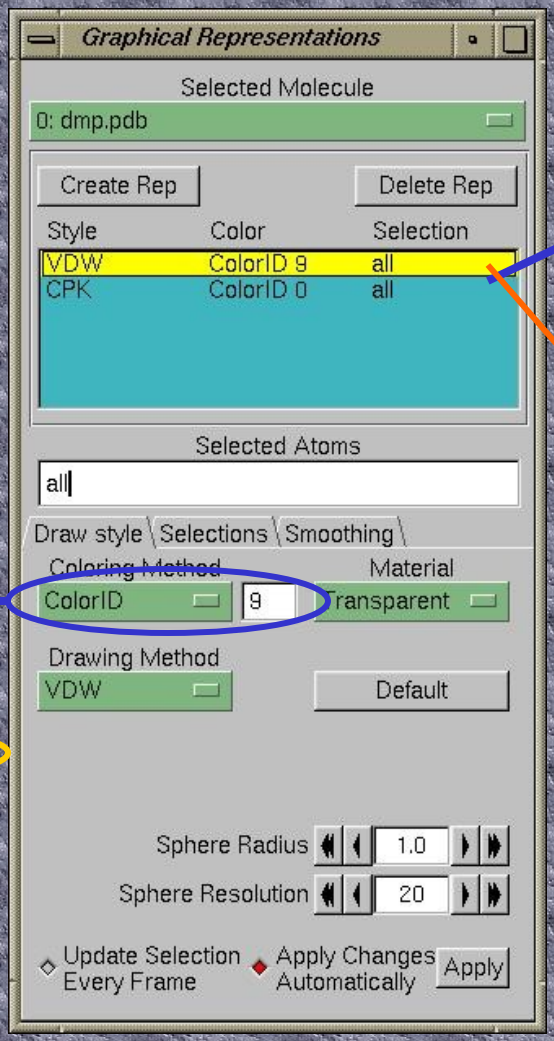








Změna barev


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
Material
ColorID
9
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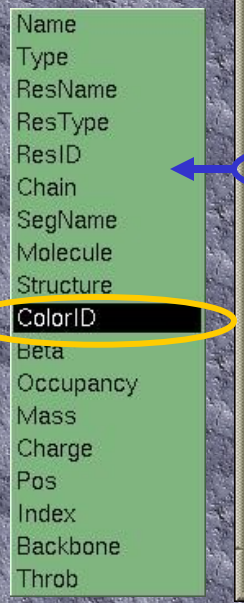
Drawing Method
VDW
Default
Sphere Radius
1.0
Sphere Resolution
20
Update Selection Every Frame
Apply Changes Automatically
Apply


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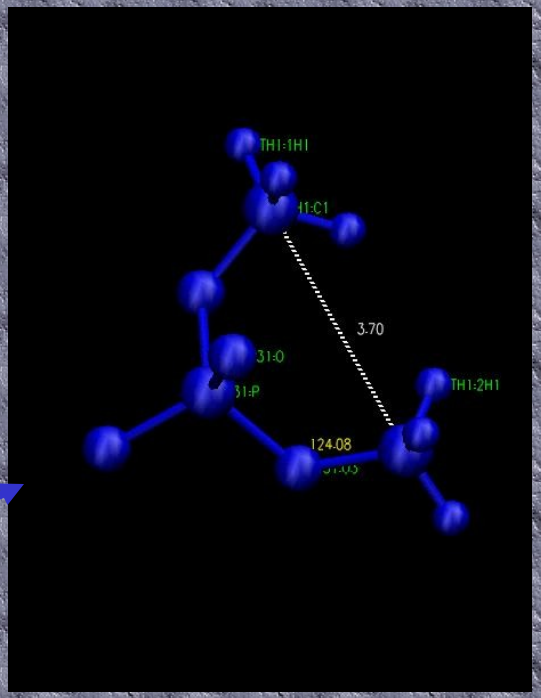
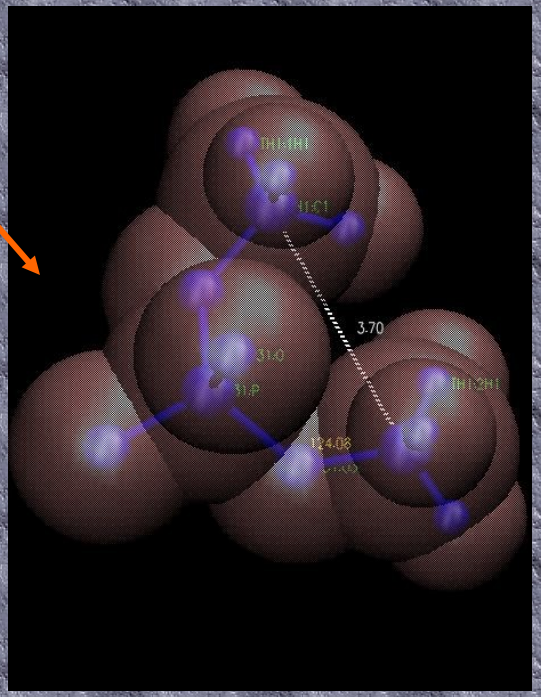
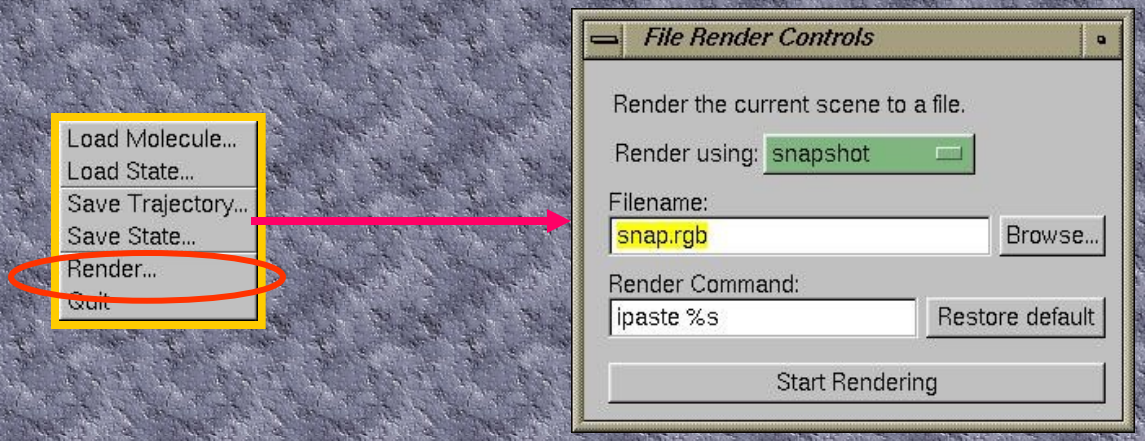
Chain
SegName
Molecule
Structure
ColorID
Beta
Occupancy
Mass
Charge
Pos
Index
Backbone
Throb

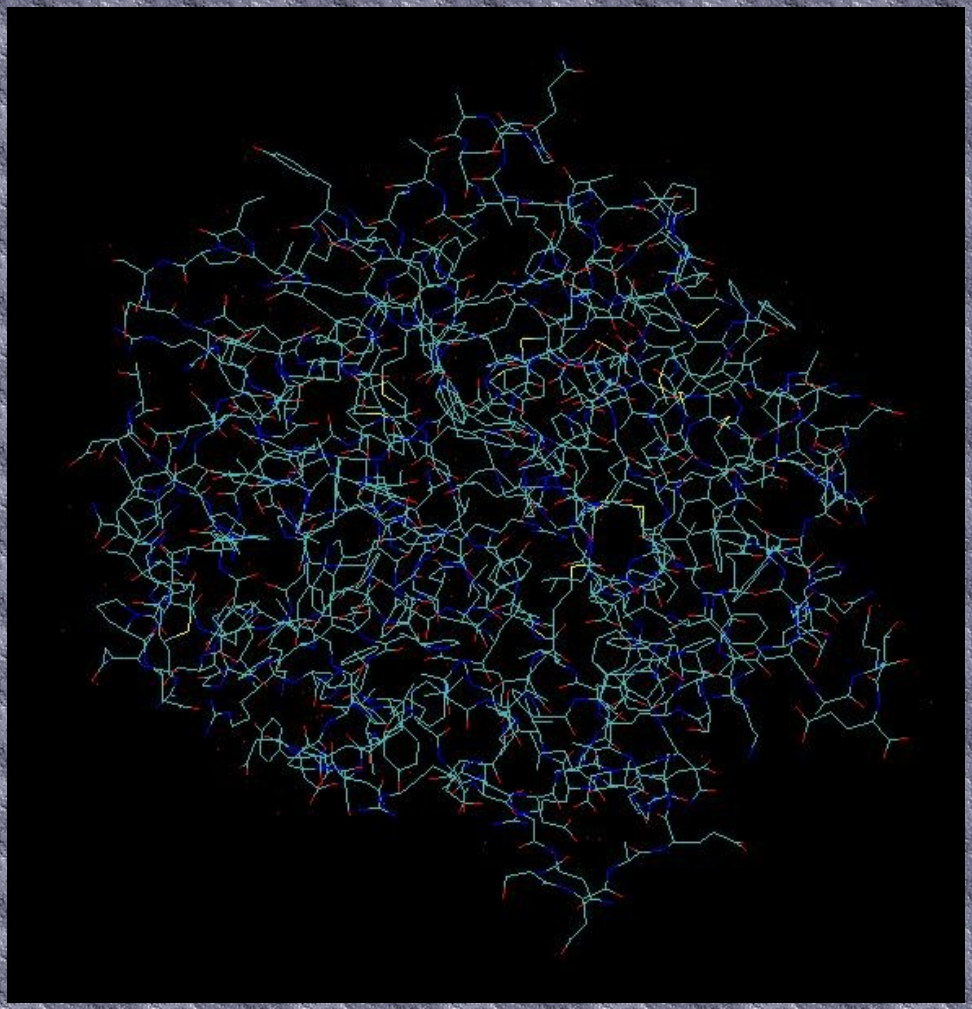

TH1:1H1
41:C1
3.70
31:O
31:P
TH1:2H1
124.08


TH1:1H1
41:C1
3.70
31:O
31:P
TH1:2H1
124.08

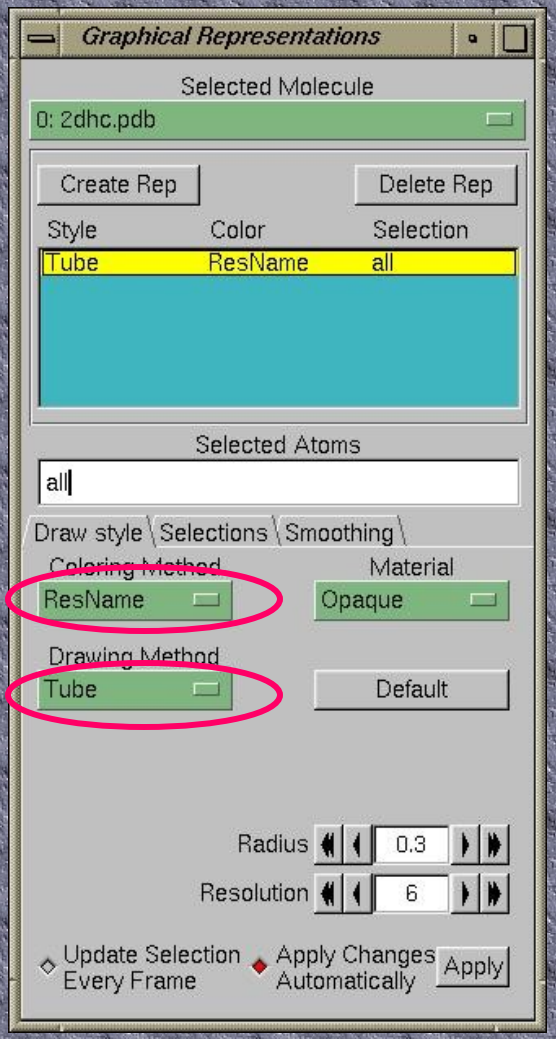
Export (uložení) obrázku

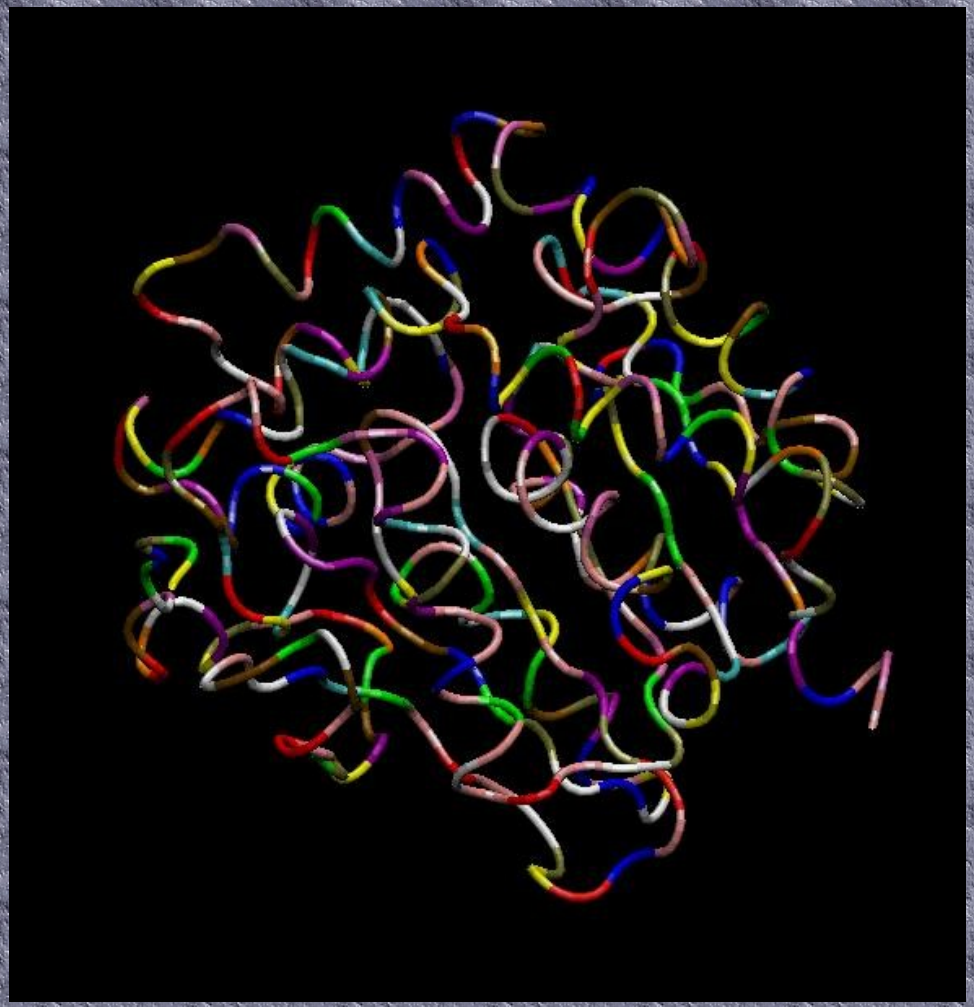


Zobrazení proteinu

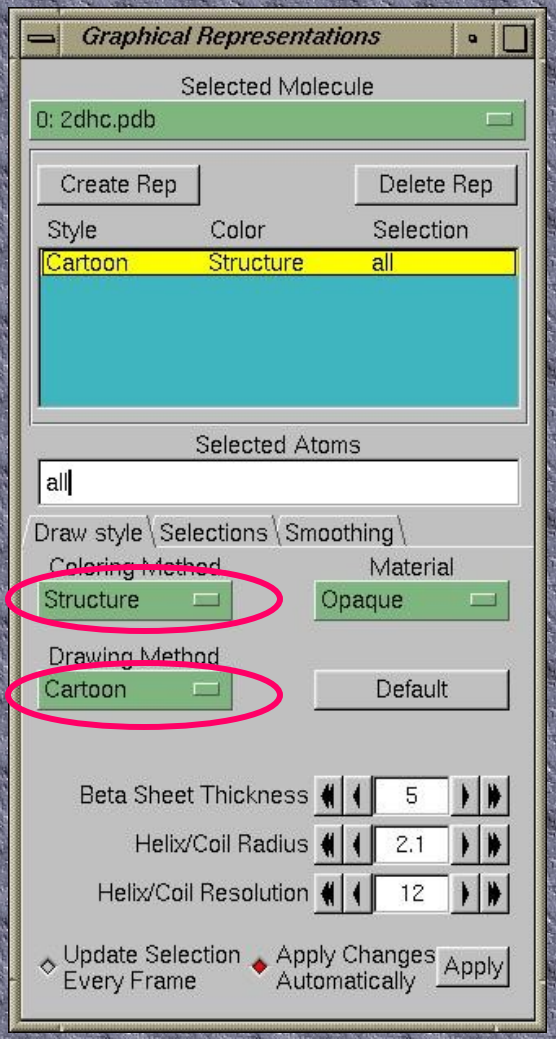


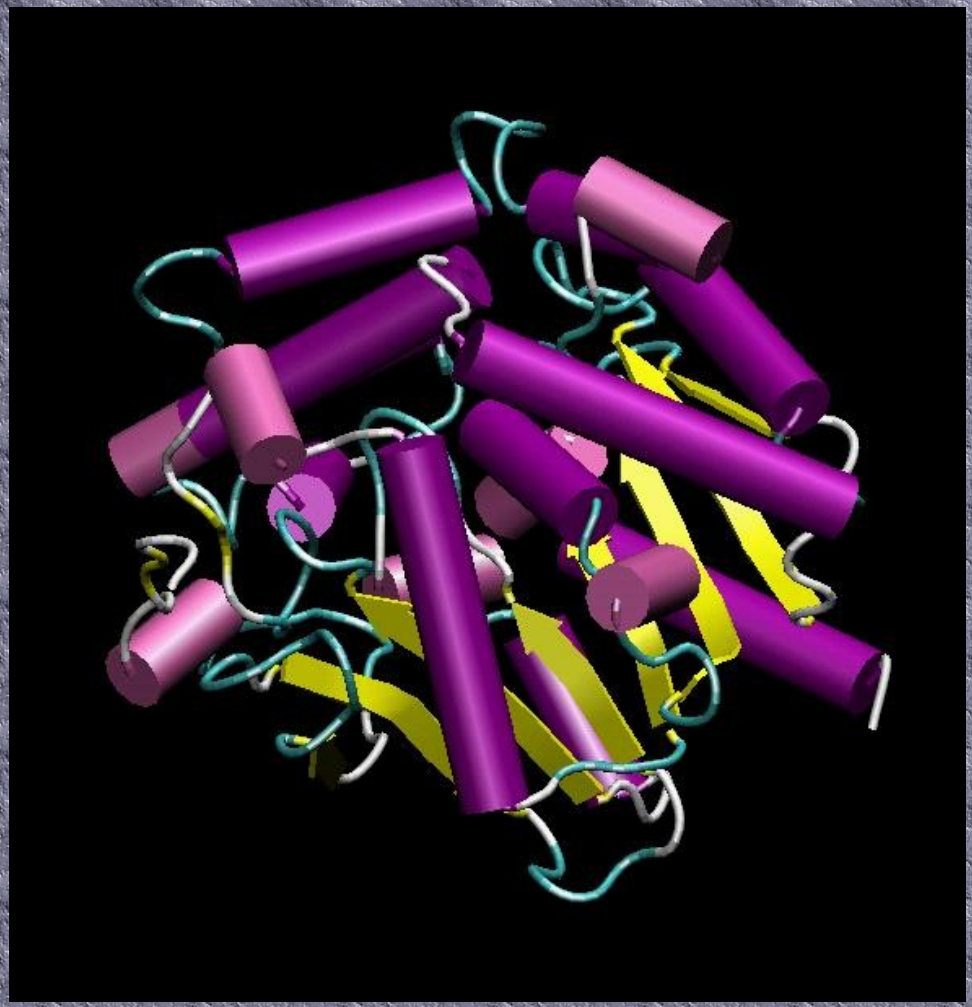
Páteř proteinu



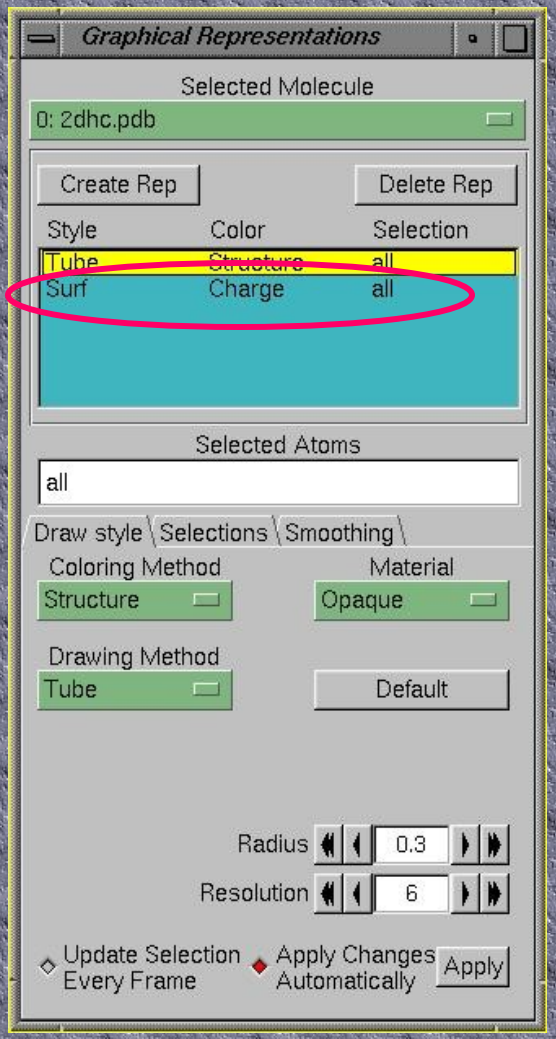


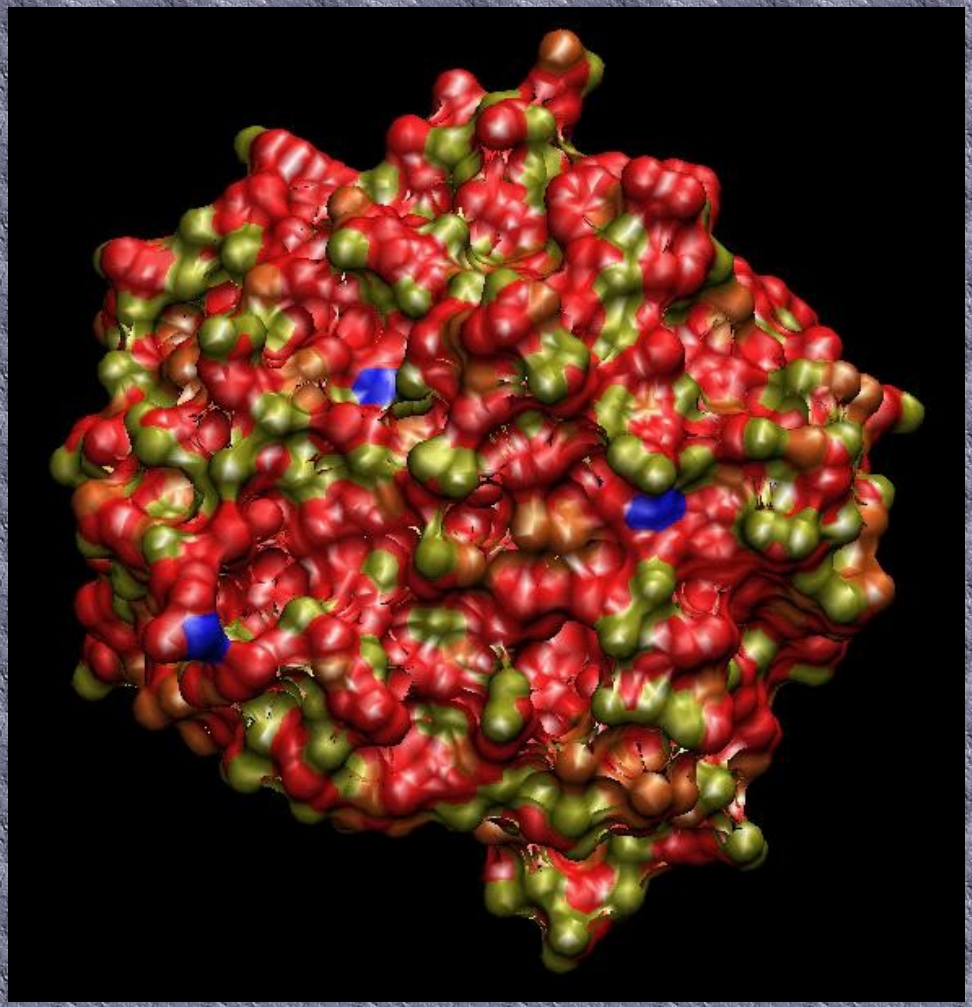
Sekundární struktury





Povrch proteinu





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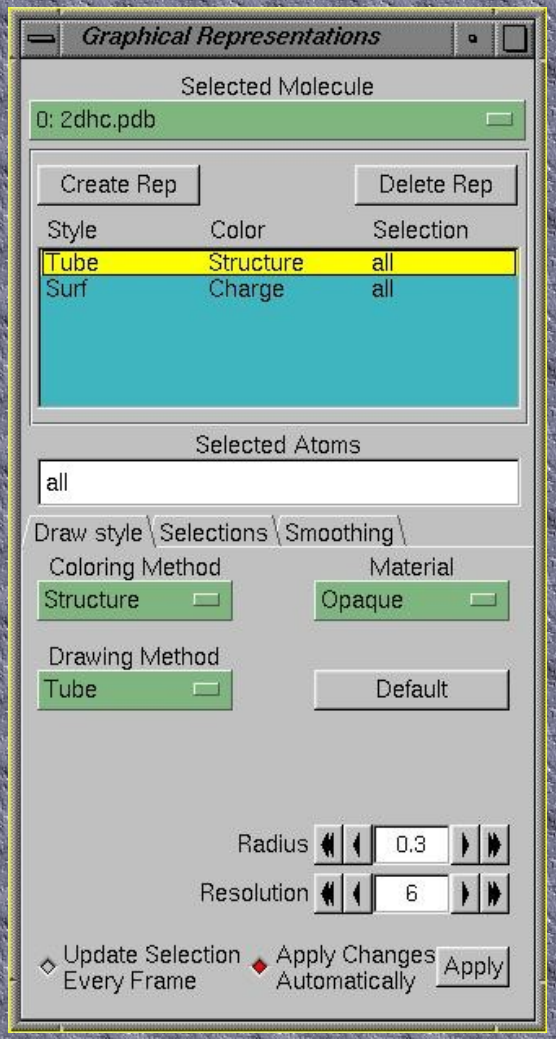
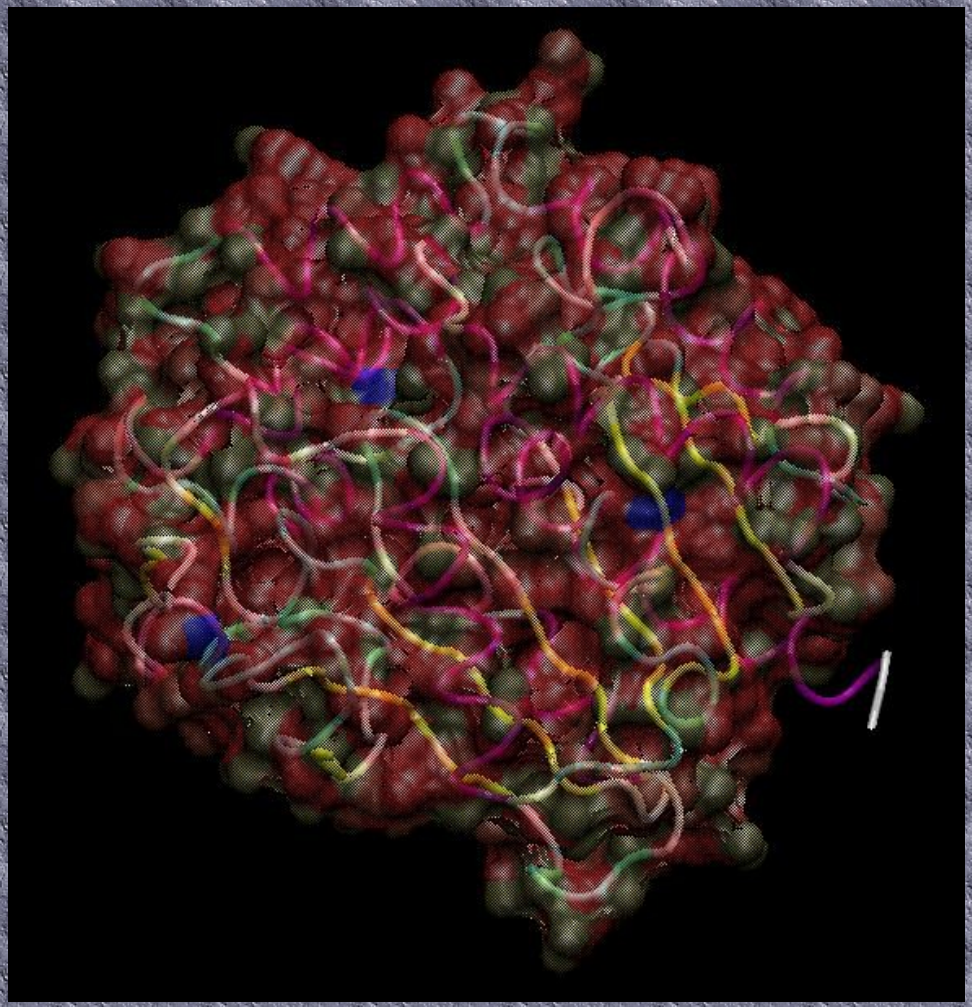




Povrchy (surfaces)

vdW povrch

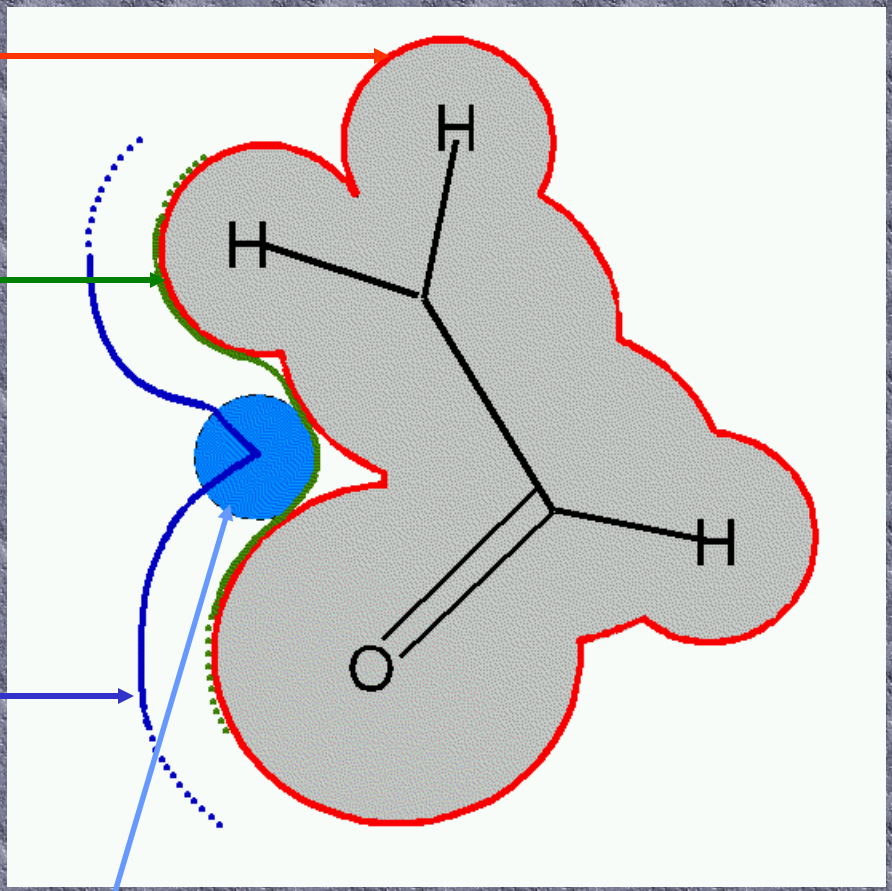
obal založený na vdW poloměrech atomů

Connolyho povrch

povrch molekuly, který je přístupný sondě o urč. poloměru

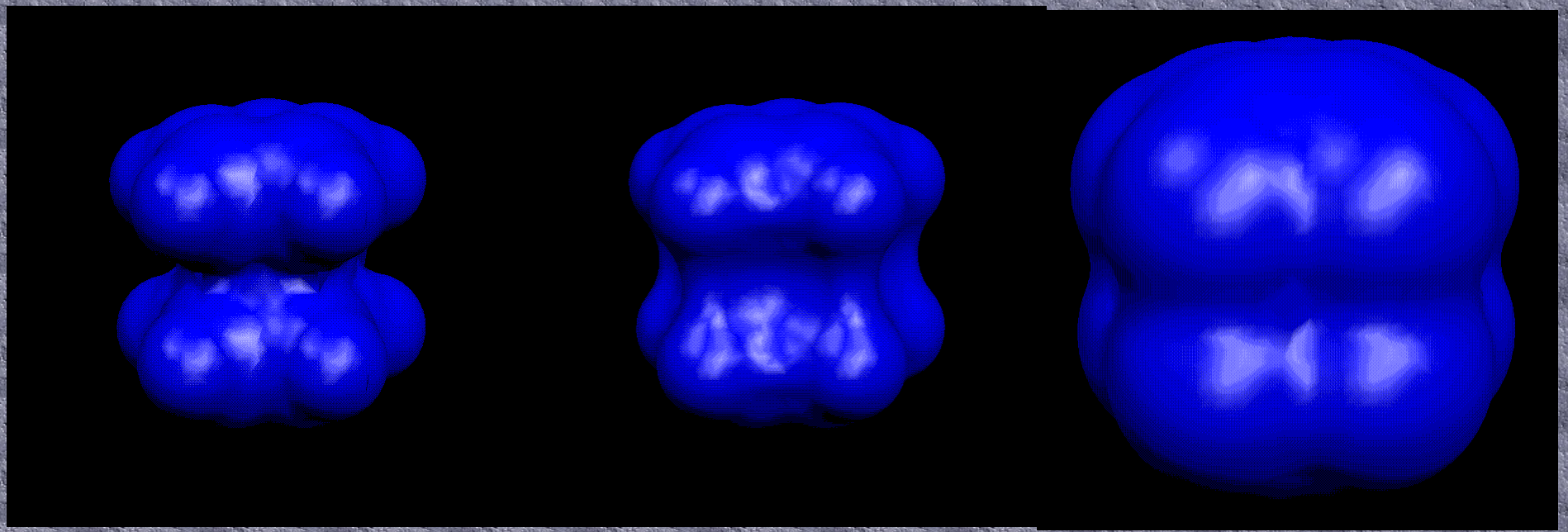
Povrch přístupný solventu = Solvent Accessible Surface Area (SASA)

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

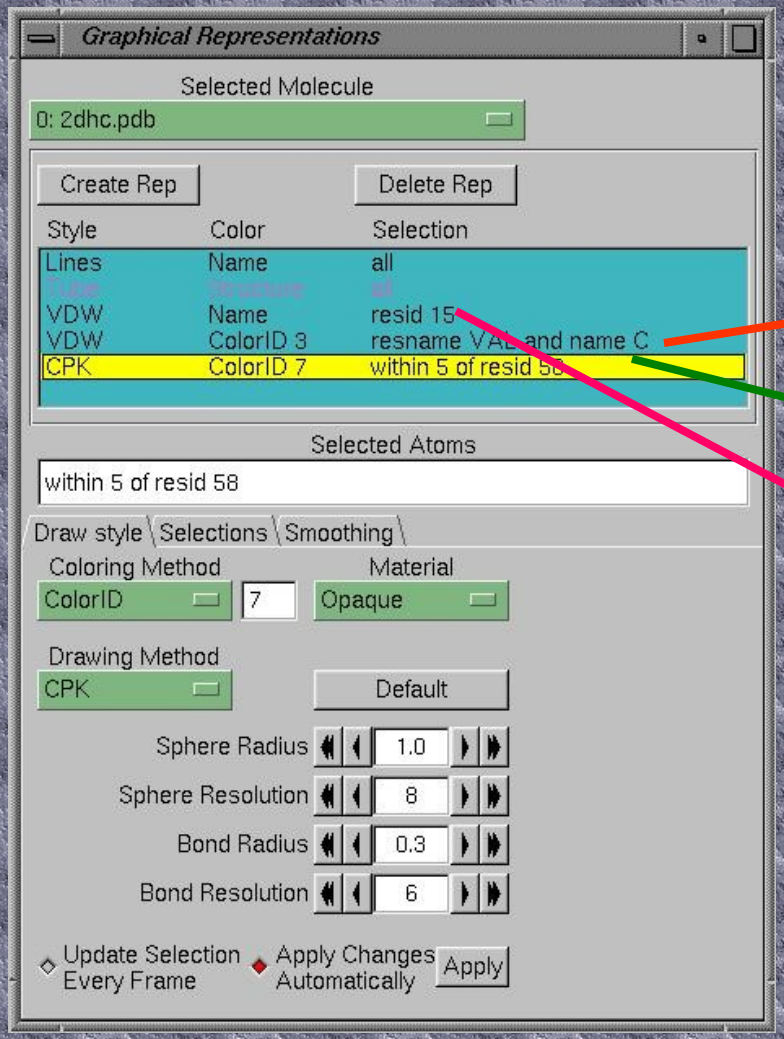


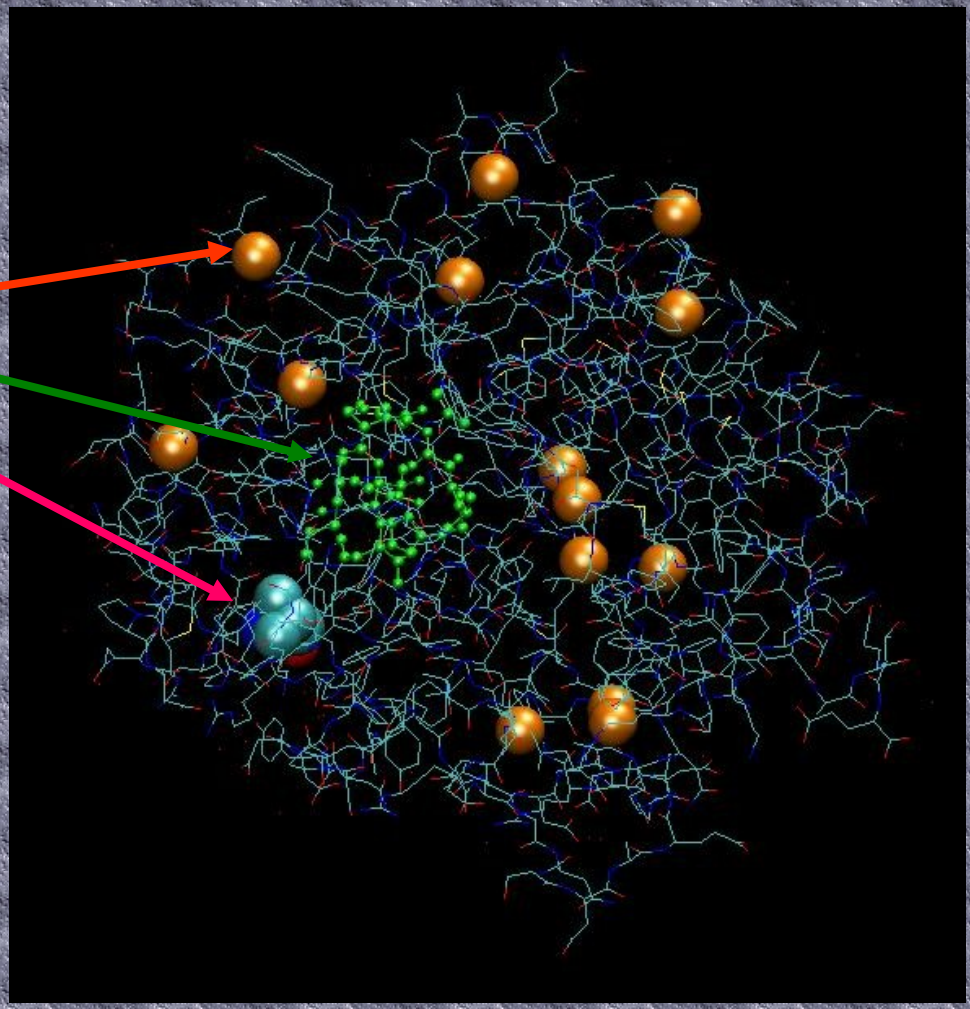
Srovnání povrchů

vdW Connolly SASA

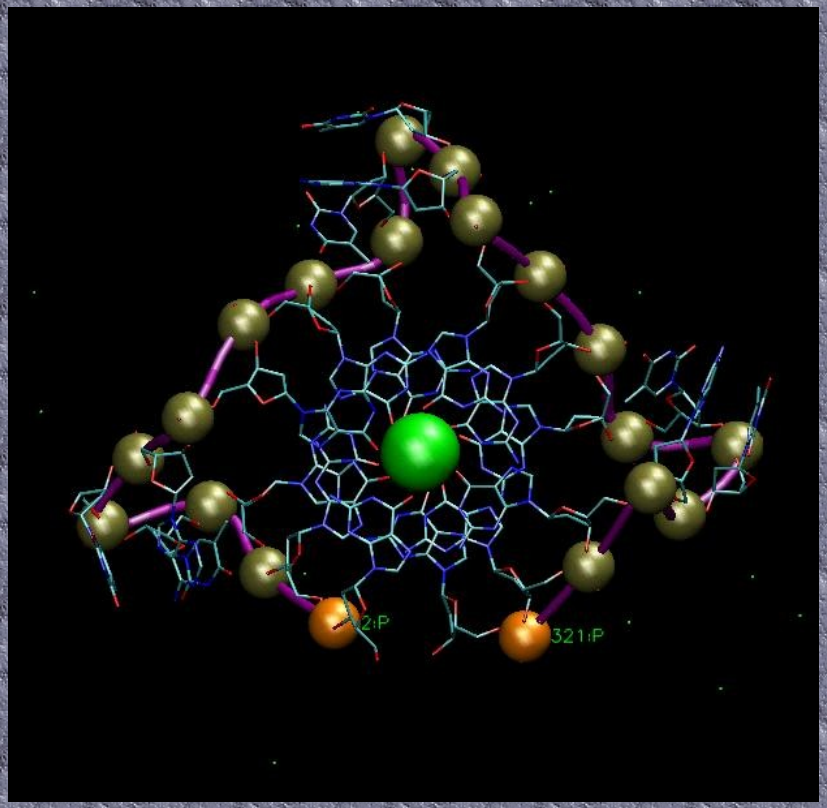


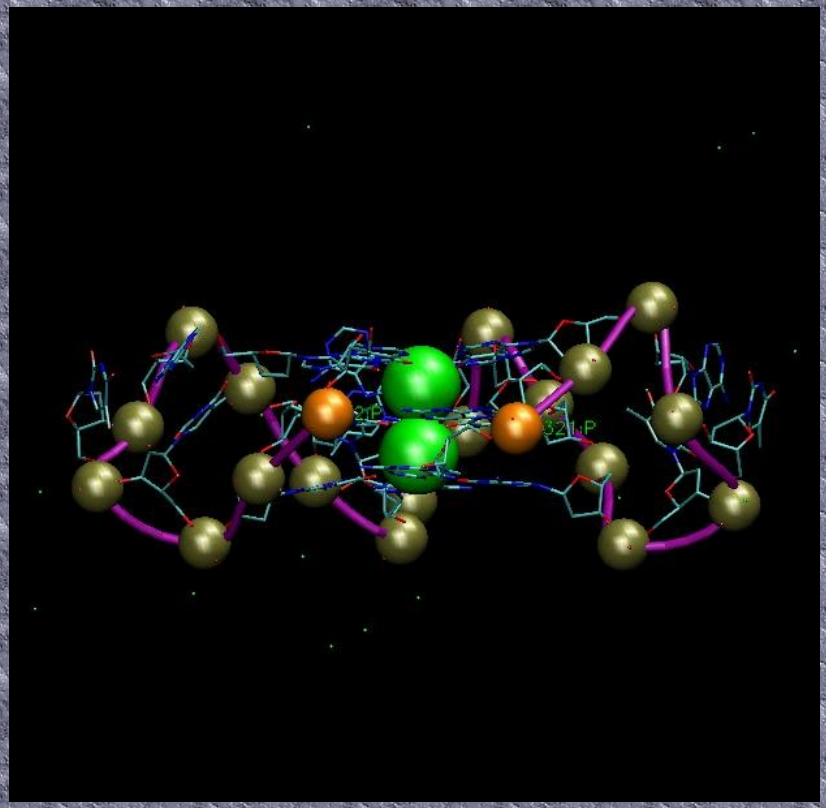
Modely vybraných částí...





Human telomere…





Cvičení…