Vizualizace molekul a strukturní databáze

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Struktura a funkce bimolekul – Letní škola – Brno, 4. - 8. září 2006

Strukturní databáze

- PDB – protein databank - http://www.pdb.org
- NDB – nucleic acids databank - http://ndbserver.rutgers.edu
- Cambridge structural database – CSD – komerční databáze organických molekul

RCSB Protein Data Bank - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://www.pdb.org/pdb/Welcome.do

English - Czech Dict... Neviditelný pes Britské listy Seznam SunSITE Czech Rep... AltaVista Technolo... Internet Christmas Ascii Pict... XXX Lookup New&Cool

RCSB PDB PROTEIN DATA BANK

A MEMBER OF THE PDB

An Information Portal to Biological Macromolecular Structures

As of Tuesday Aug 22, 2006 there are 38320 Structures | PDB Statistics

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- Educational Resources
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- General Information
- Acknowledgements
- Frequently Asked Questions
- Known Problems
- Report Bugs/Comments

Welcome to the RCSB PDB

The RCSB PDB provides a variety of tools and resources for studying the structures of biological macromolecules and their relationships to sequence, function, and disease.

The RCSB is a member of the wwPDB whose mission is to ensure that the PDB archive remains an international resource with uniform data.

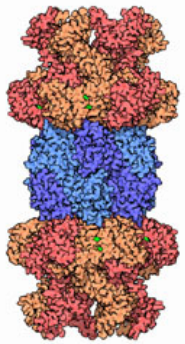
This site offers tools for browsing, searching, and reporting that utilize the data resulting from ongoing efforts to create a more consistent and comprehensive archive.

Information about compatible browsers can be found here.

A narrated tutorial illustrates how to search, navigate, browse, generate reports and visualize structures using this new site. [This requires the Macromedia Flash player download.]

Comments? info@rcsb.org

Molecule of the Month: AAA+ Proteases



How would you make a protein cutting machine that would be safe to use inside a cell? Digestive proteases like trypsin and pepsin are small and efficient–they diffuse up to proteins and start cutting. This would never work inside a cell. The cell needs to have more control, so that only obsolete or damaged proteins are destroyed. The AAA+ proteases are one solution to this problem. They use two tricks to ensure that only certain proteins are destroyed. First, they hide the protein destruction machinery inside a closed container, and second, they use a special protein pump to feed proteins into this destruction chamber.

- More ...
- Previous Features

NEWS

- Complete News
- Newsletter
- Discussion Forum

22-August-2006

RCSB PDB Poster Prize Awarded at ACA and ECM Meetings

Thanks to everyone who participated in the recent RCSB PDB Poster Prize competitions for best student poster related to macromolecular crystallography. Prizes were awarded at the July ACA meeting in Hawaii and the August EC Meeting in Belgium.

- Full Story ...

15-August-2006

Phasing Out Theoretical Model Depositions to the PDB Archive

Done

Inbox for zdenek@chemi... vizualizace.odp - OpenOffi... xosview

RCSB Protein Data Ban... zdenek@bubo [11]

14:24

WELCOME TO THE NUCLEIC ACID DATABASE

a repository of three-dimensional structural information about nucleic acids

- Atlas
- Deposit Data
- Download Data
- Search
- Reports
- Education
- Standards
- Tools
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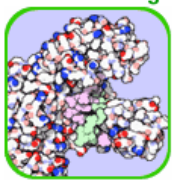
Number of Released Structures:
3176 Structures
Last Update: 15-August-2006

Search the NDB by ID
Enter an NDB ID or PDB ID
Search
Search for Released Structures

Nucleic Acids Highlight



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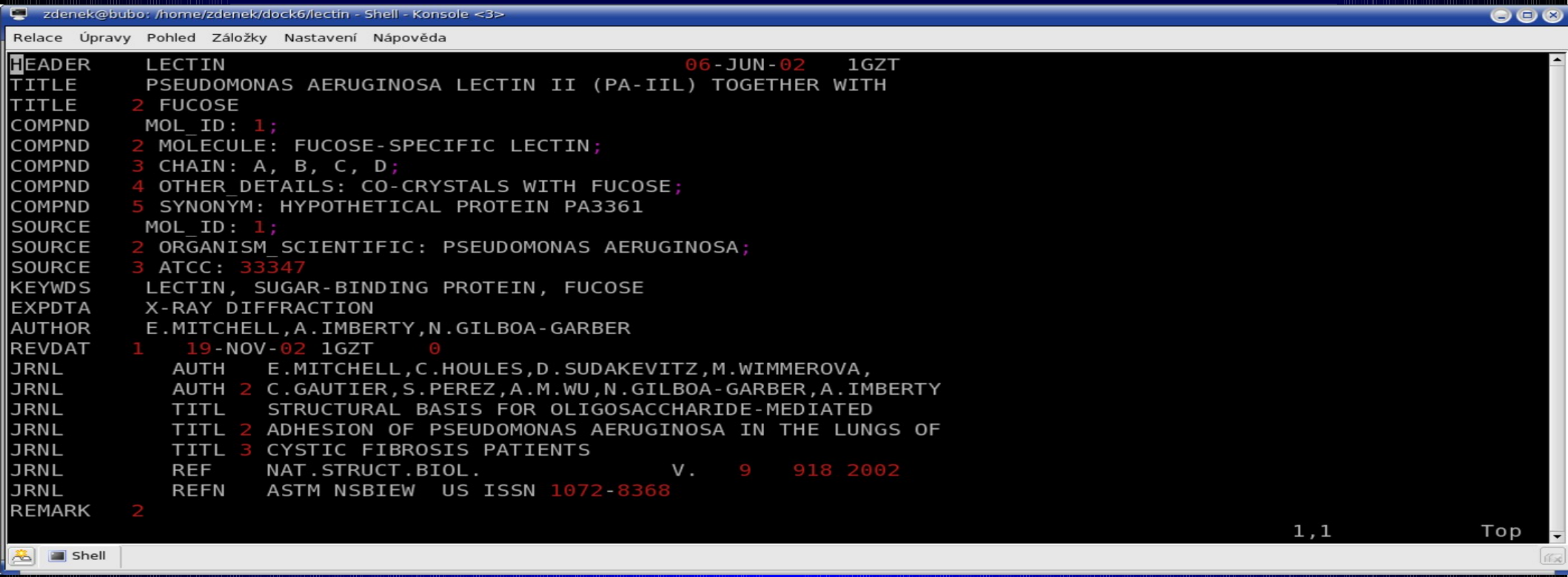
The NDB is supported by funds from the National Science Foundation and the Department of Energy.

In citing the NDB please refer to: H. M. Berman, W. K. Olson, D. L. Beveridge, J. Westbrook, A. Gelbin, T. Demeny, S.-H. Hsieh, A. R. Srinivasan, and B. Schneider. (1992) The Nucleic Acid Database: A Comprehensive Relational Database of Three-Dimensional Structures of Nucleic Acids. Biophys. J., 63, 751-759.

ndbadmin@ndbserver.rutgers.edu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TITLE 2 FUCOSE
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COMPND 2 MOLECULE: FUCOSE-SPECIFIC LECTIN;
COMPND 3 CHAIN: A, B, C, D;
COMPND 4 OTHER_DETAILS: CO-CRYSTALS WITH FUCOSE;
COMPND 5 SYNONYM: HYPOTHETICAL PROTEIN PA3361
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SOURCE 2 ORGANISM_SCIENTIFIC: PSEUDOMONAS AERUGINOSA;
SOURCE 3 ATCC: 33347
KEYWDS LECTIN, SUGAR-BINDING PROTEIN, FUCOSE
EXPDTA X-RAY DIFFRACTION
AUTHOR E.MITCHELL,A.IMBERTY,N.GILBOA-GARBER
REVDAT 1 19-NOV-02 1GZT 0
JRNL AUTH E.MITCHELL,C.HOULES,D.SUDAKEVITZ,M.WIMMEROVA,
JRNL AUTH 2 C.GAUTIER,S.PEREZ,A.M.WU,N.GILBOA-GARBER,A.IMBERTY
JRNL TITL STRUCTURAL BASIS FOR OLIGOSACCHARIDE-MEDIATED
JRNL TITL 2 ADHESION OF PSEUDOMONAS AERUGINOSA IN THE LUNGS OF
JRNL TITL 3 CYSTIC FIBROSIS PATIENTS
JRNL REF NAT.STRUCT.BIOL. V. 9 918 2002
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REMARK 2
1,1 Top
Shell


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ATOM 18 CG GLN A 3 15.768 17.691 45.147 1.00 4.98 C
ATOM 19 CD GLN A 3 15.448 19.080 44.648 1.00 5.35 C
ATOM 20 OE1 GLN A 3 14.788 19.234 43.600 1.00 10.08 O
ATOM 21 NE2 GLN A 3 15.882 20.067 45.365 1.00 4.27 N
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ATOM 24 C GLY A 4 20.311 16.141 40.078 1.00 5.52 C
ATOM 25 O GLY A 4 21.339 15.626 39.652 1.00 6.49 O
ATOM 26 N VAL A 5 19.182 16.211 39.394 1.00 5.79 N
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ATOM 28 C VAL A 5 18.797 16.903 37.108 1.00 6.06 C
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ATOM 32 CG2 VAL A 5 18.202 13.462 38.732 1.00 8.45 C
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ATOM 35 C PHE A 6 19.540 17.665 33.670 1.00 7.47 C
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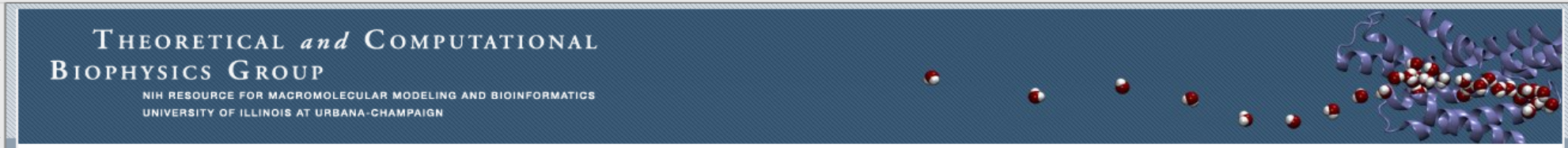
ATOM 37 CB PHE A 6 20.662 19.083 35.350 1.00 5.89 C
ATOM 38 CG PHE A 6 20.844 19.477 36.775 1.00 5.89 C
ATOM 39 CD1 PHE A 6 20.014 20.392 37.378 1.00 6.62 C
631,1 12%

Programy pro vizualizaci molekul

- Freeware
  - VMD
  - Rasmol
  - Pymol
  - Chimera
- Komerční
  - InsightII
  - Sybyl
  - Spartan

Program VMD

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



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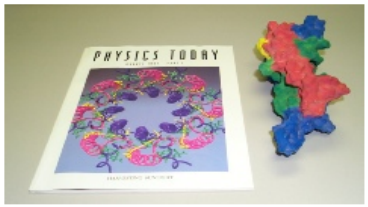
VMD
Visual Molecular Dynamics

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. VMD supports computers running MacOS-X, Unix, or Windows, is distributed free of charge, and includes source code.
(more details...)

Spotlight

VMD can be used with 3-D printers to create solid models of molecular structures such as the LH-II heterodimer unit shown at right. The most recent version of VMD supports the newest color-capable 3-D printers, and can generate STL or VRML files suitable for 3-D printing. Two identical LH-II heterodimer units were printed in 6.4 hours on a Z-Corp Z400 3-D printer at an approximate cost of $1 to $2 per cubic inch. Each of the two solid models consumed 12.4 cubic inches of the ZP102 powder.
Other Spotlights



Overview

Molecular representations
Supported molecular file formats
Interactive molecular dynamics
Required software
Programs that use VMD
VMD publications
How to cite VMD, Papers citing VMD

Download

Download (all versions)
VMD 1.8.5 (MacOS-X, Unix, Windows)
VMD 1.8.4 (MacOS-X, Unix, Windows)
VMD plugin library
VMD script library
License, Copyright and Disclaimer

Documentation and Support

User and installation guides
Quick help
FAQ

News and Announcements

VMD 1.8.5 (MacOS-X, Unix, Windows) (8/25/2006) NEW
A paper describing the new MultiSeq plugin included in VMD 1.8.5 has been published in BMC Bioinformatics (8/16/2006) NEW
The 2006 VMD User Survey is now complete (8/21/2006)
VMD image "highly commended" in Concepts category of the 2005 Visions of Science Photographic Awards
CatDCD trajectory processor version 4.0 released
Past announcements

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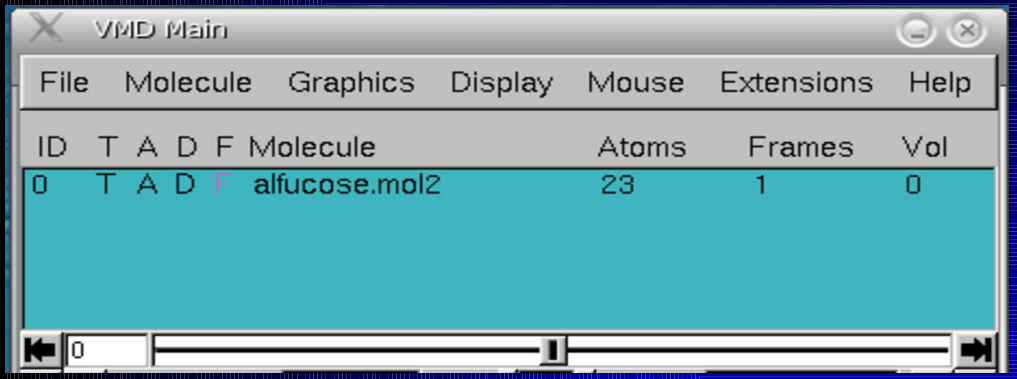
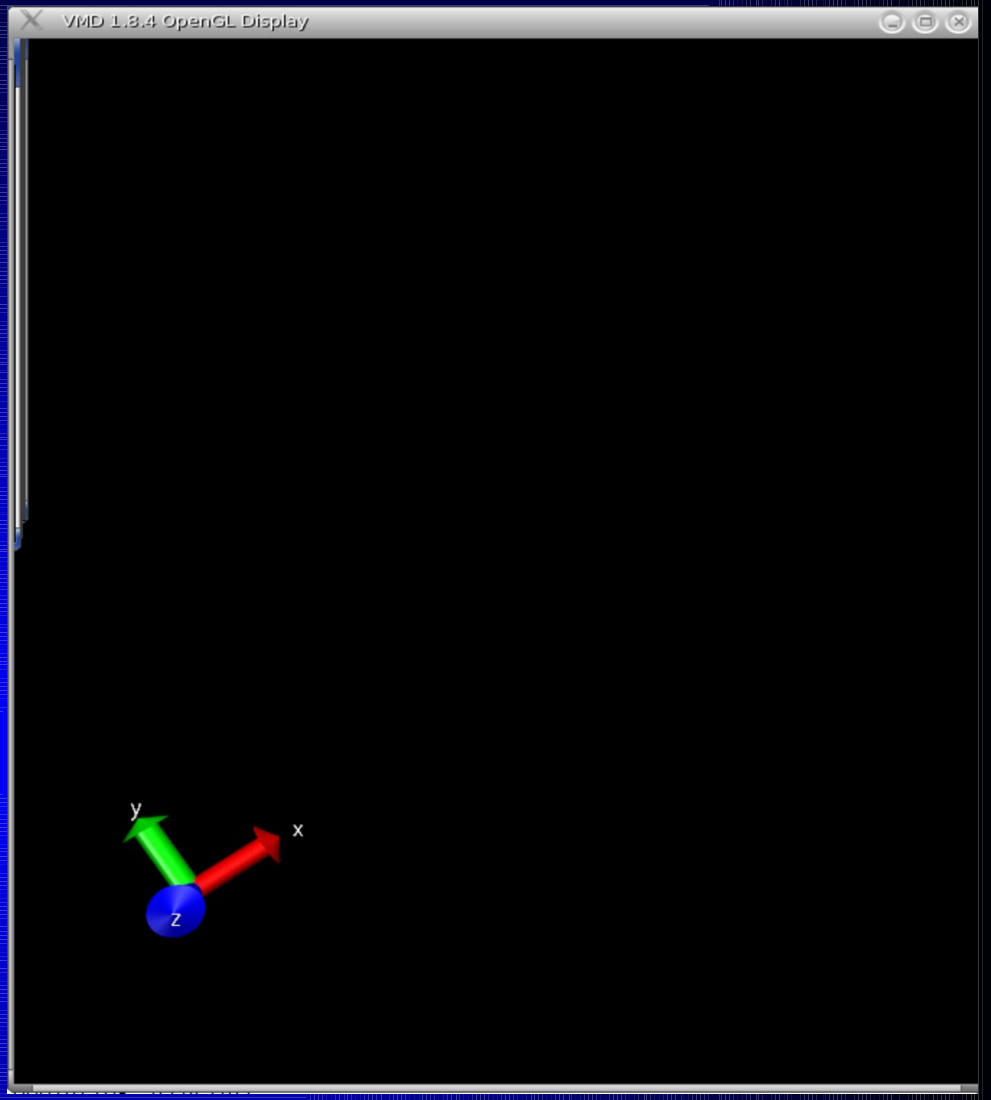
Brochure

Development

2003 VMD User Survey Results
VMD development status and pre-release test downloads
CVS source code access
Bug tracking database

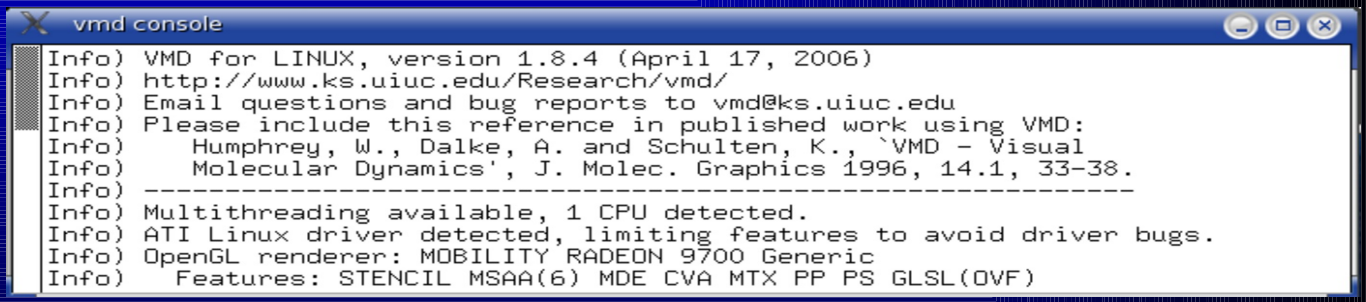


Hlavní panel

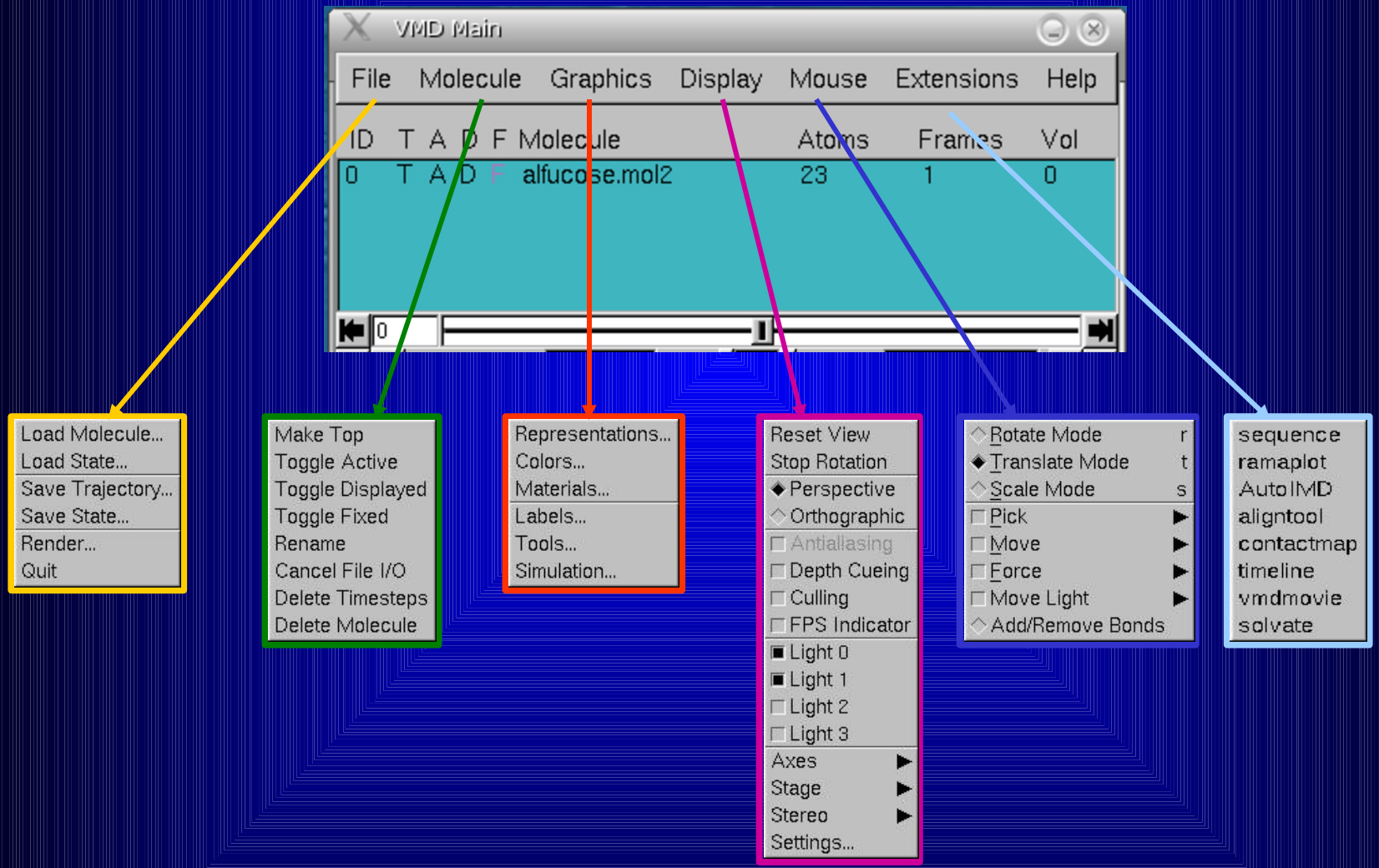


Display

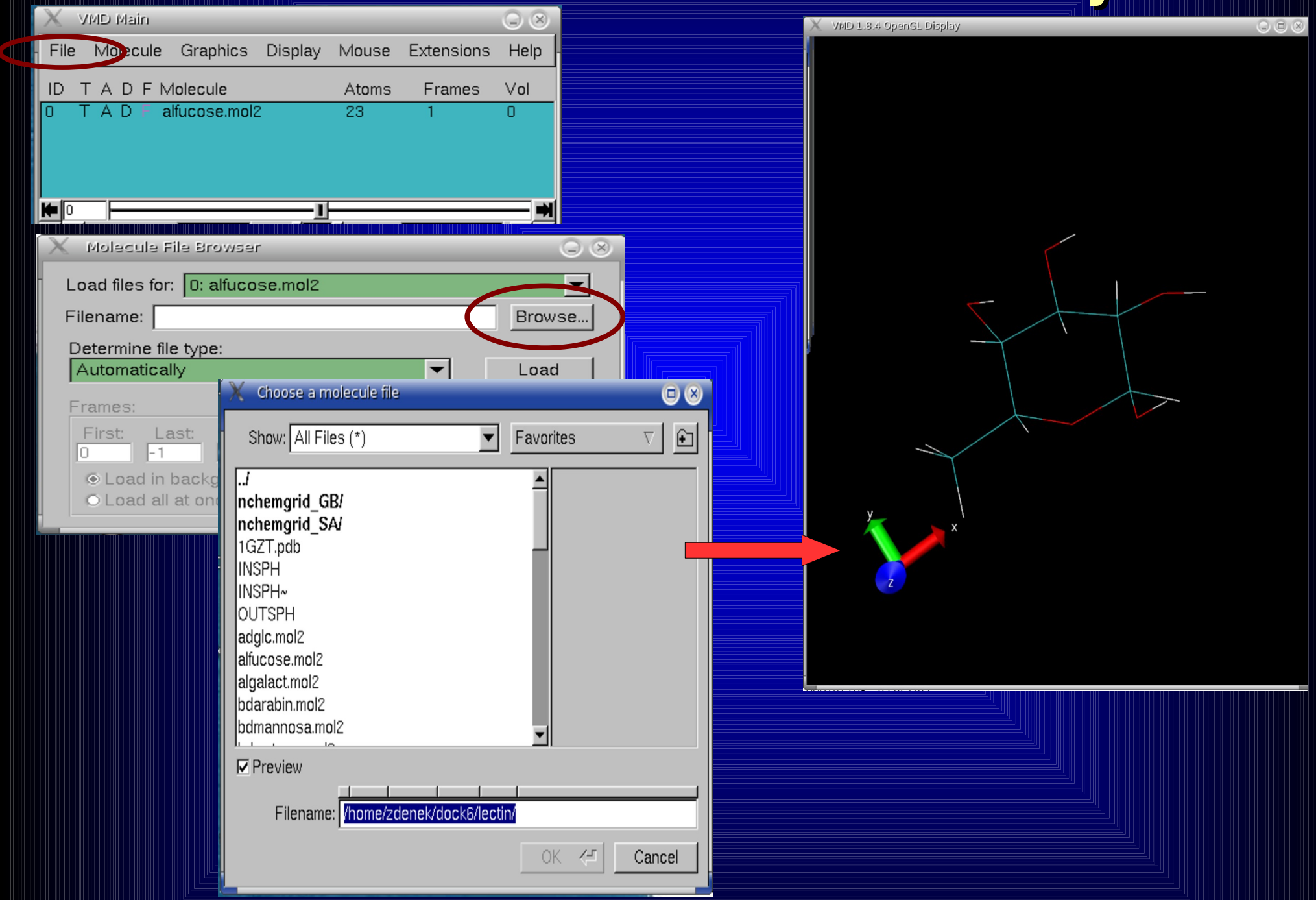
Textový terminál



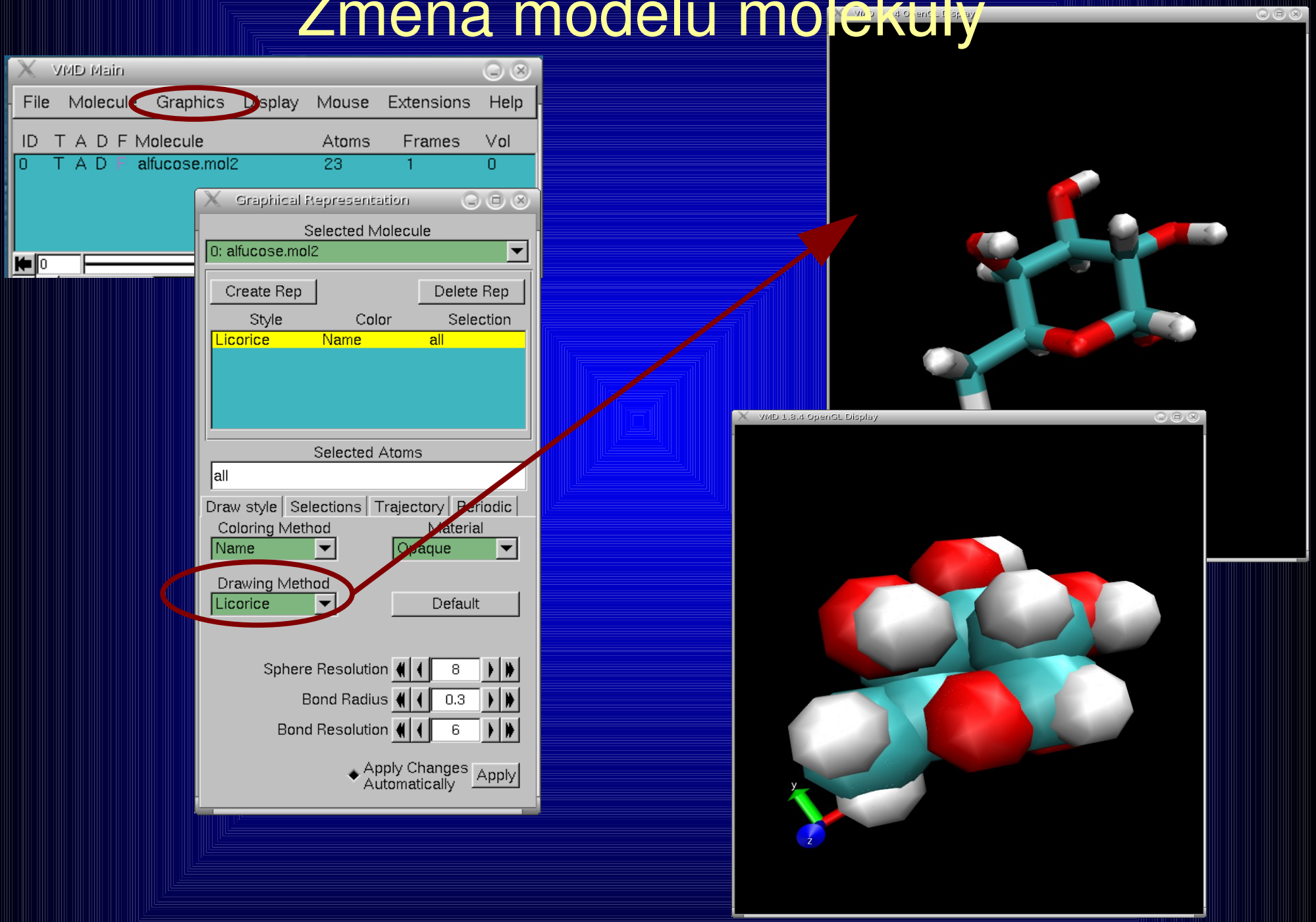
VMD – hlavní panel



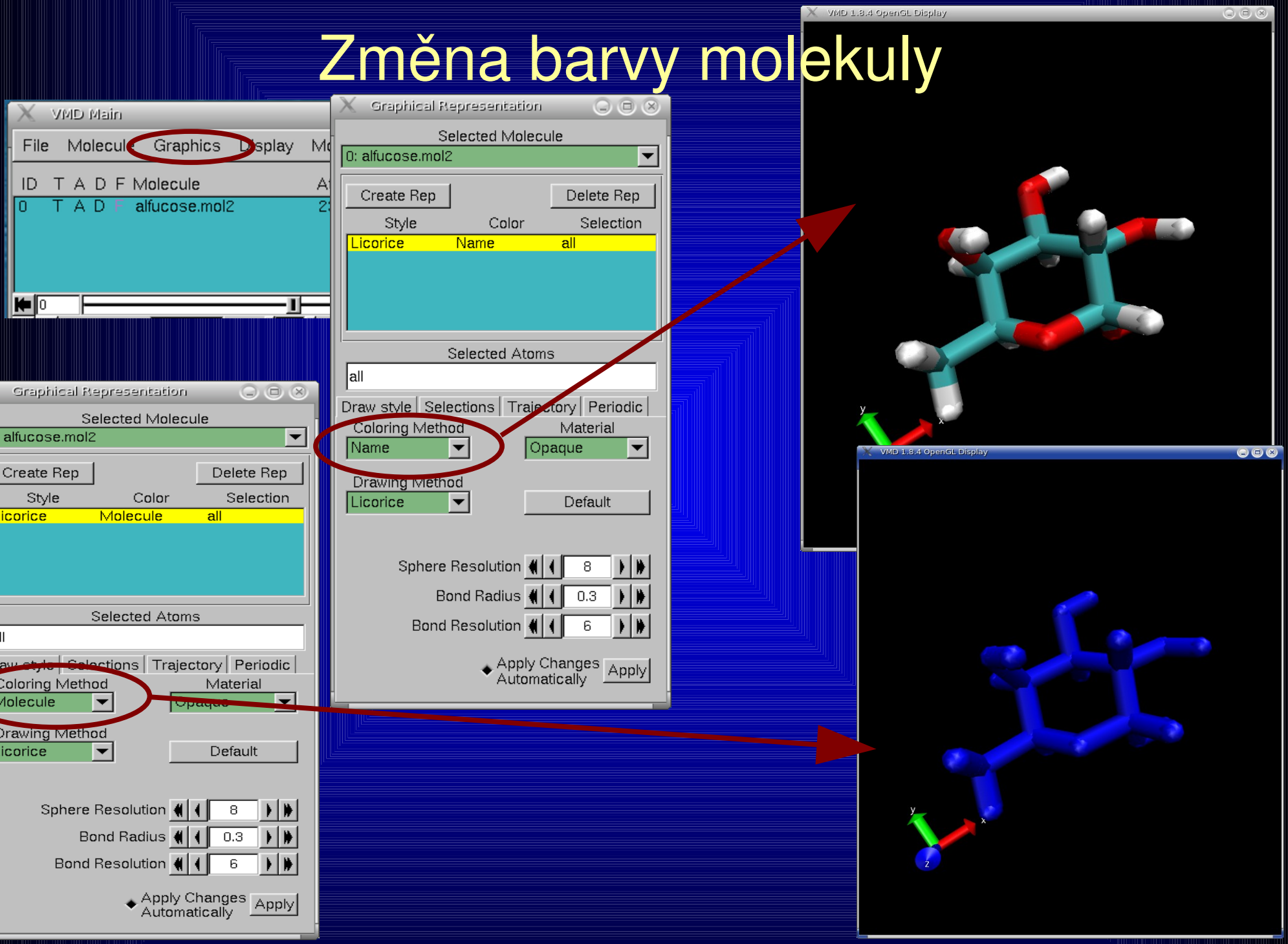
Načtení souřadnic molekuly



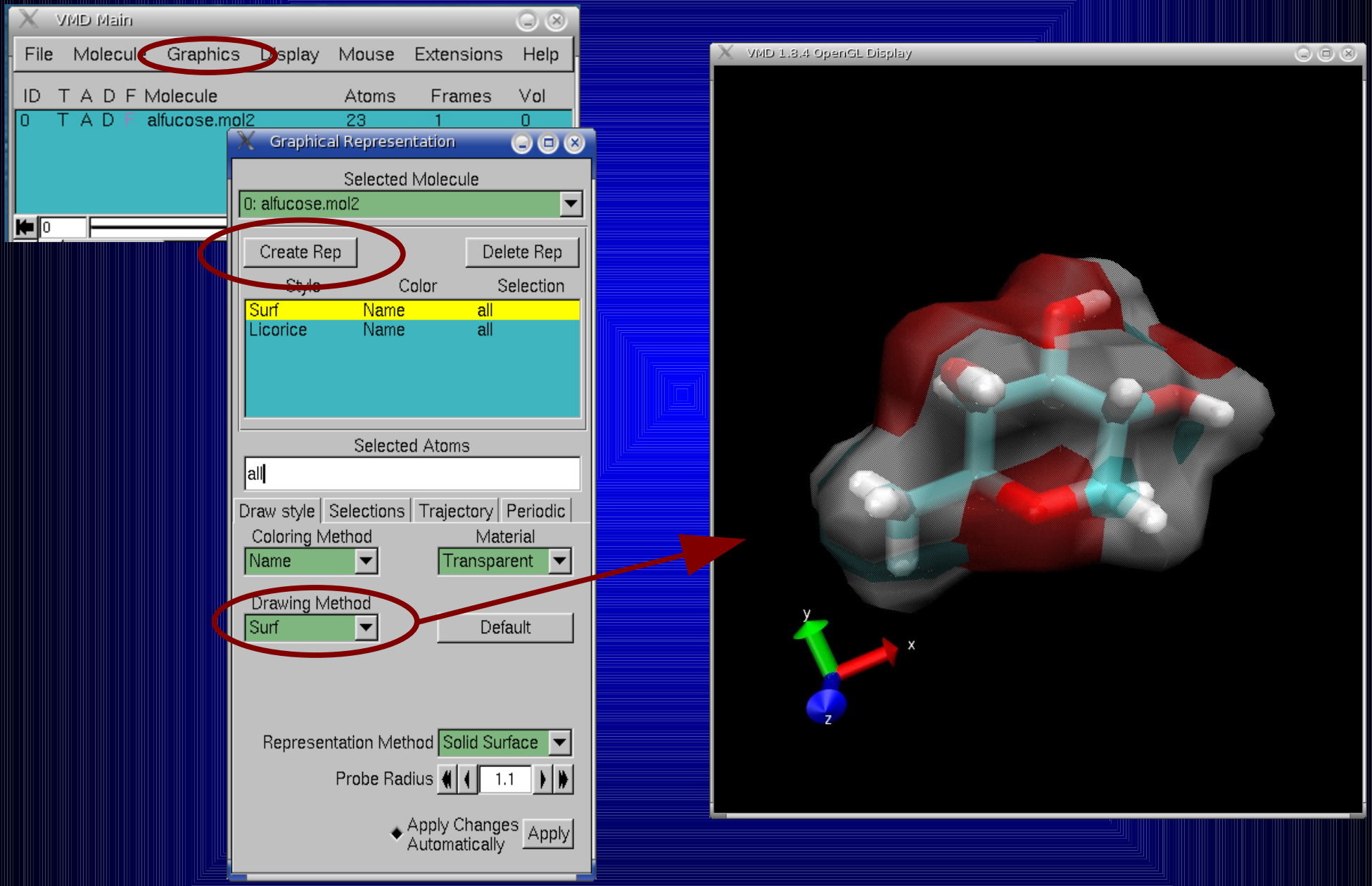
Změna modelu molekuly



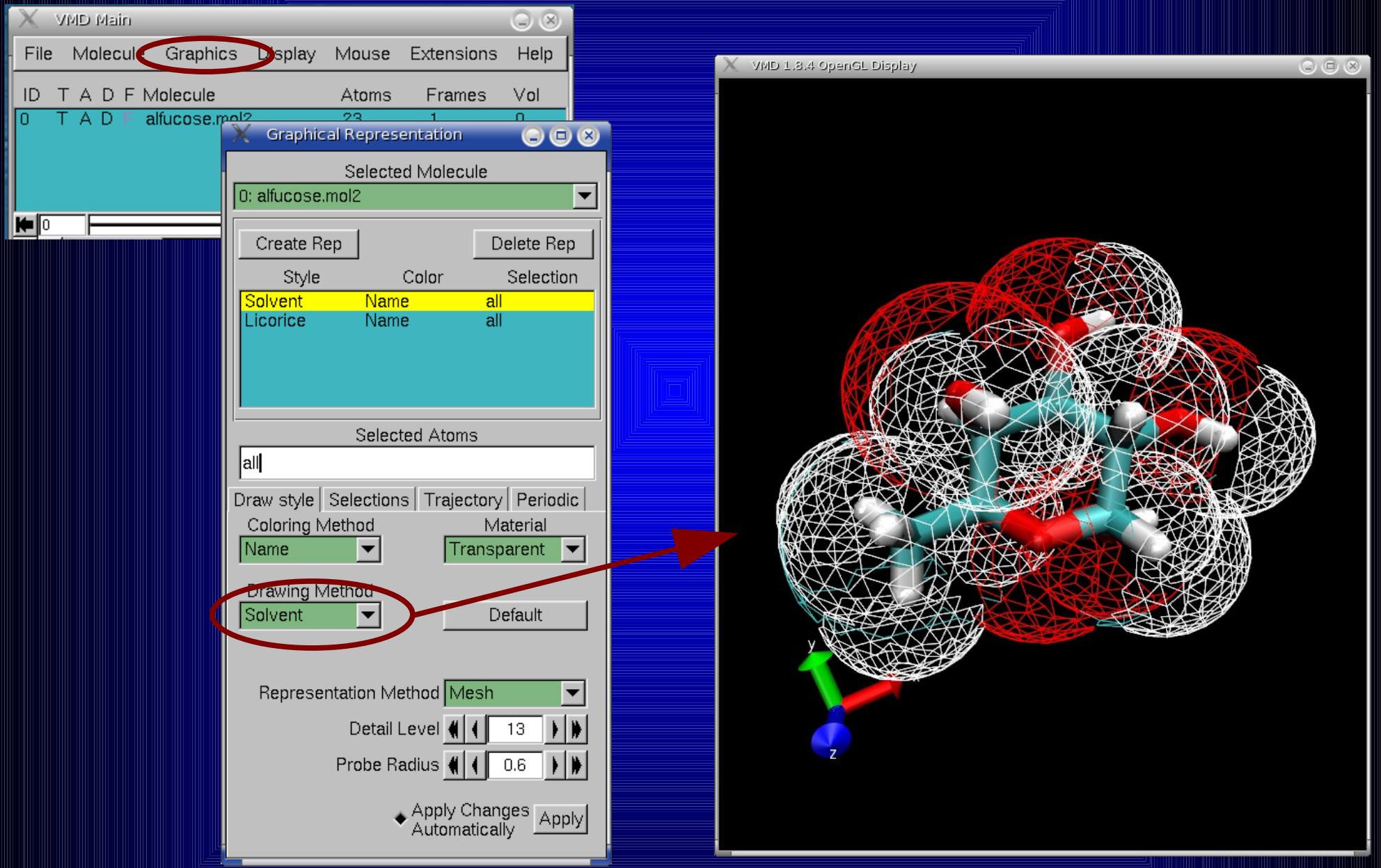
Změna barvy molekuly



Povrch molekuly



Povrch molekuly přístupný solventu



Povrchy molekul

vdW povrch

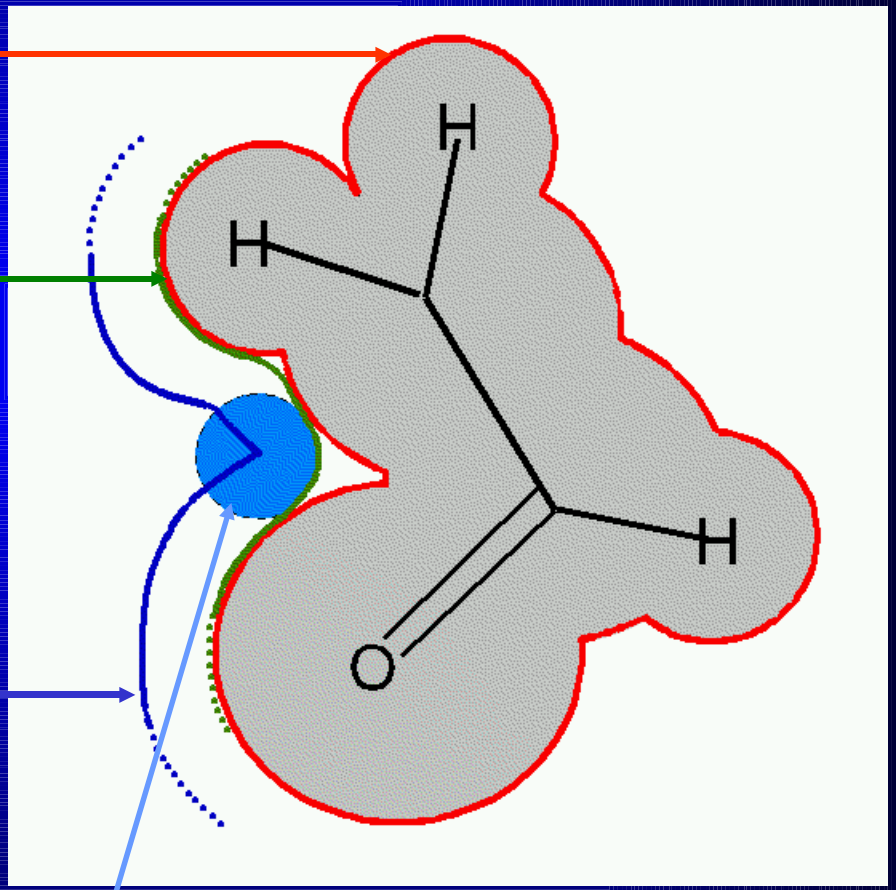
obal založený na vdW poloměrech atomů

Connolyho povrch

povrch molekuly, který je přístupný sondě o urč. poloměru

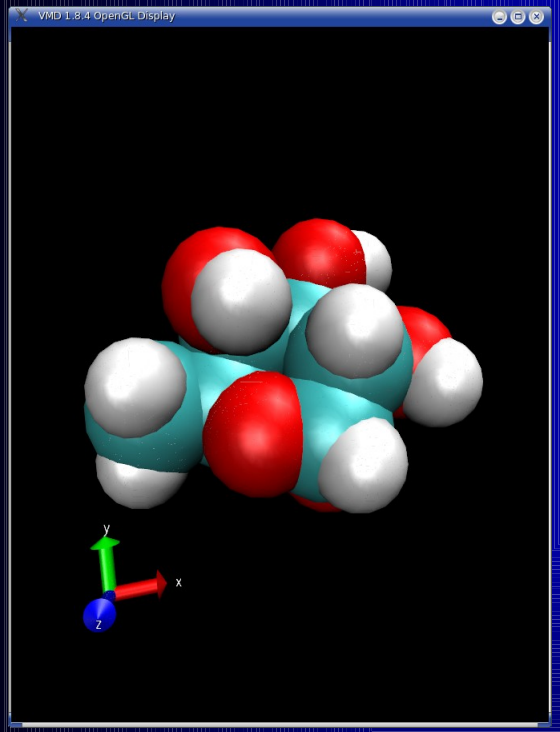
Povrch přístupný solventu = Solvent Accessible Surface Area (SASA)

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

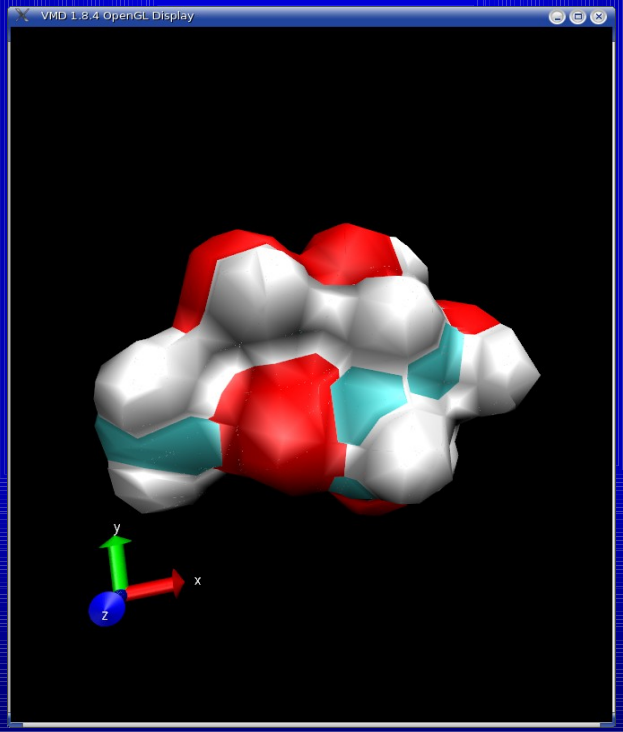


Povrchy molekul - srovnání

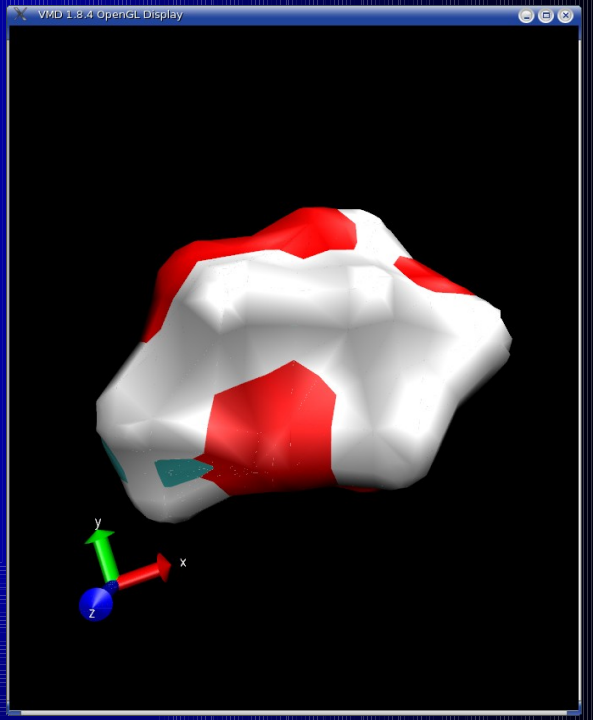
vdW



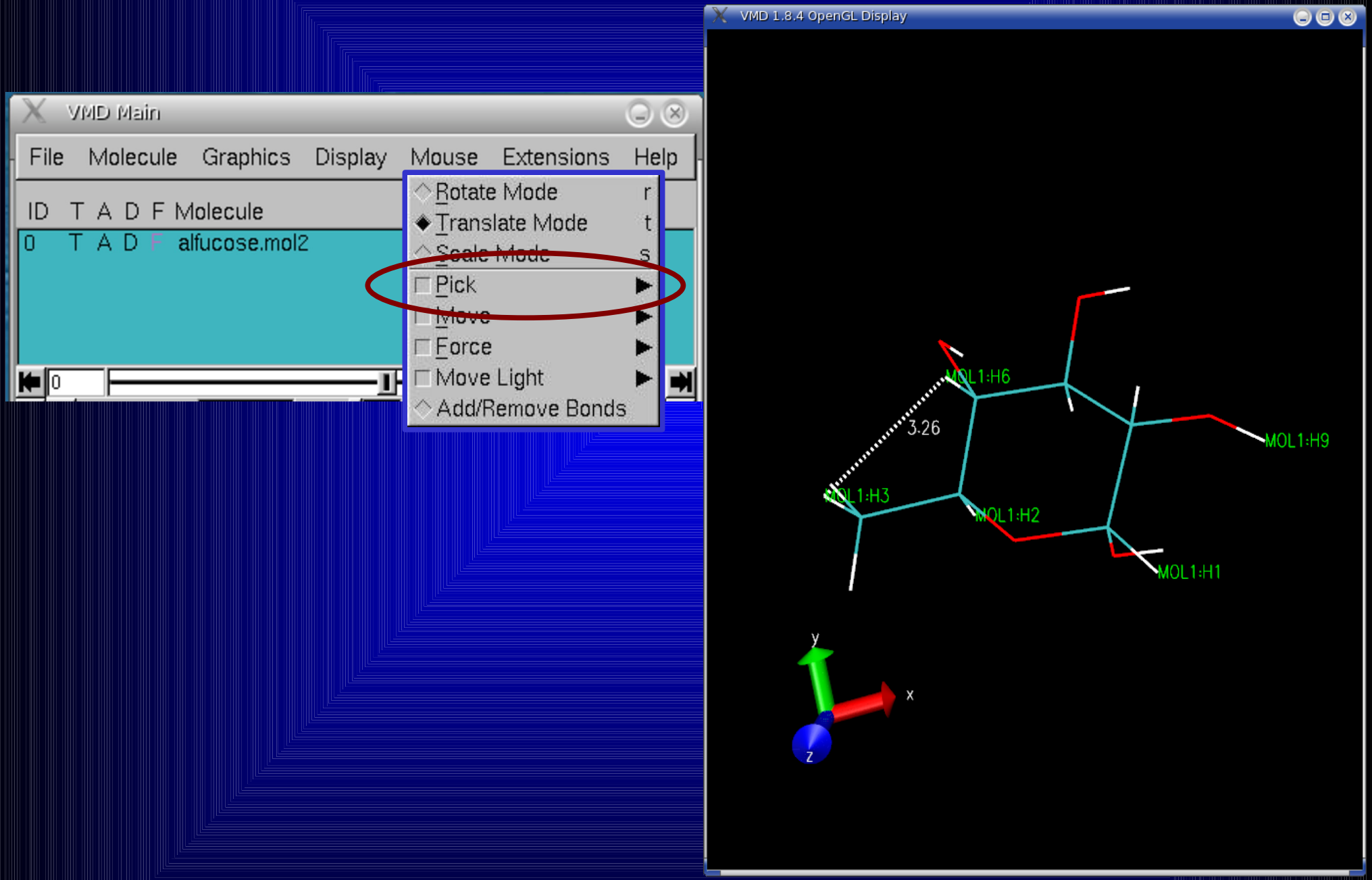
Connolly



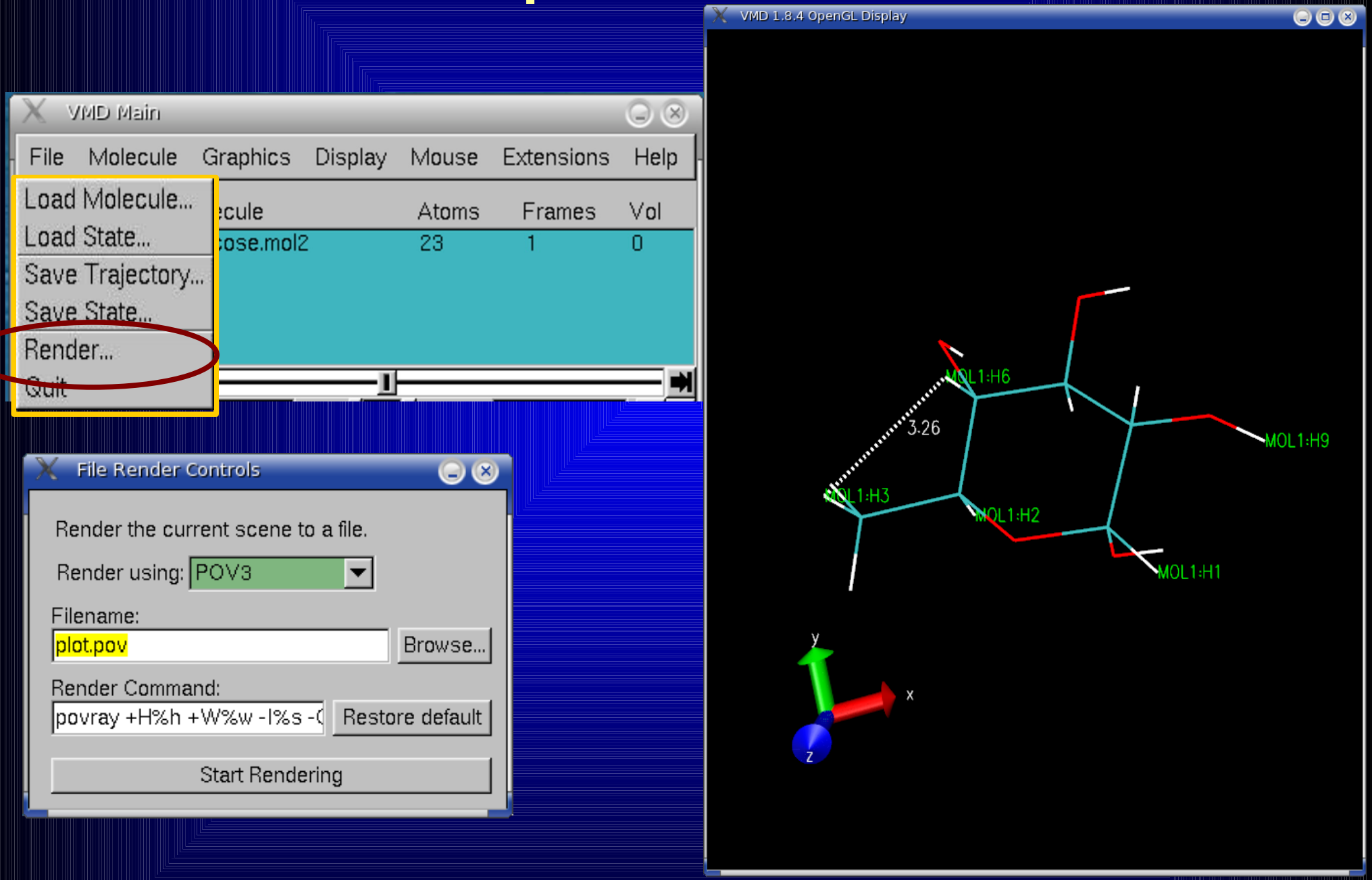
SASA



Měření vzdáleností, úhlů ....



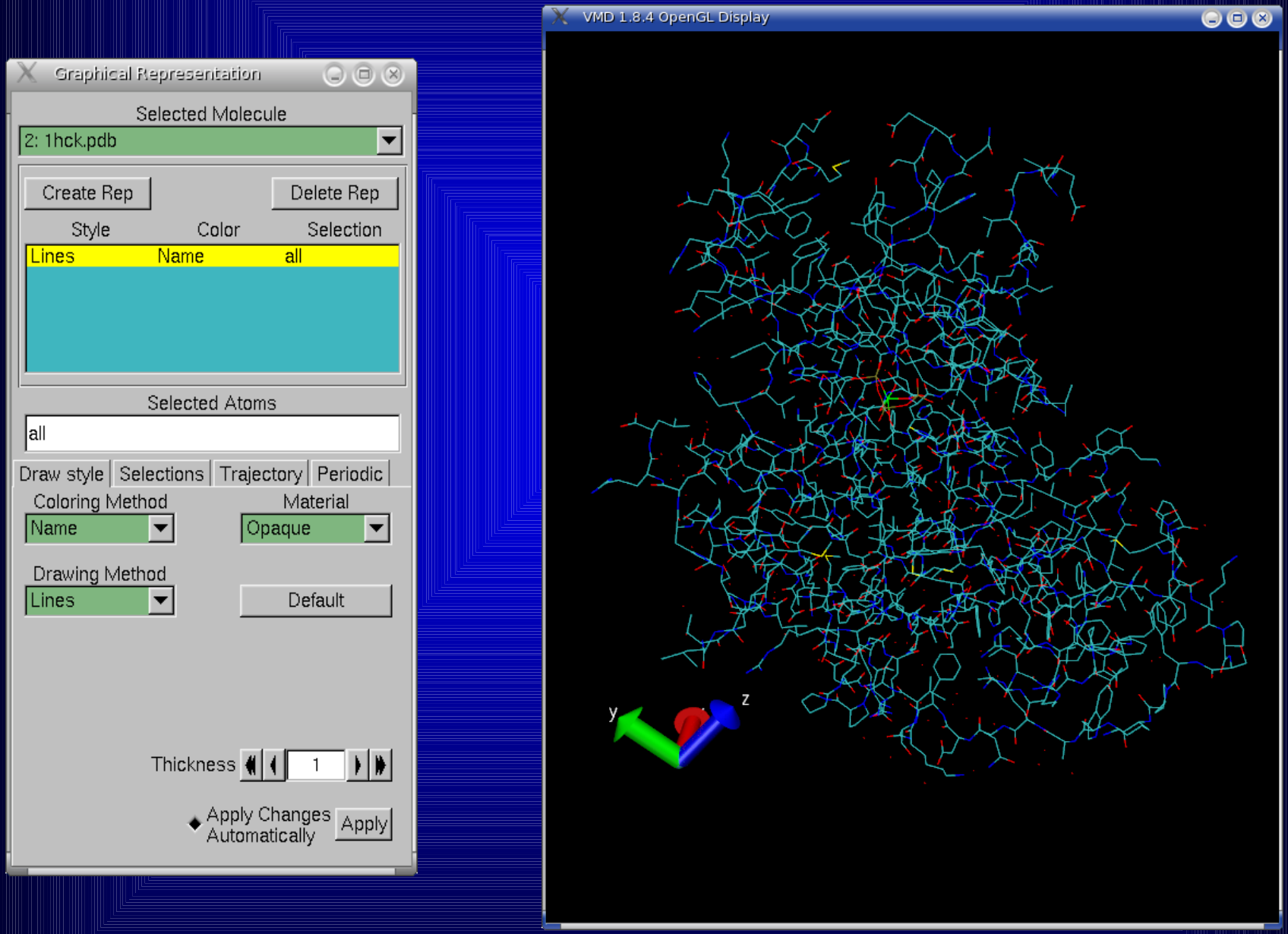
Export obrázku



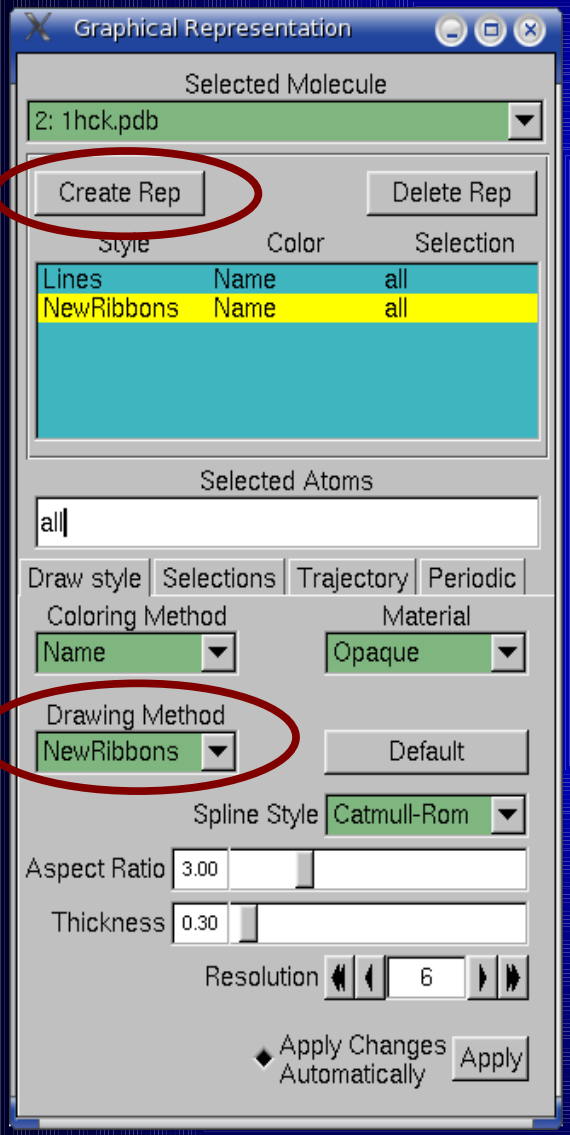
VMD

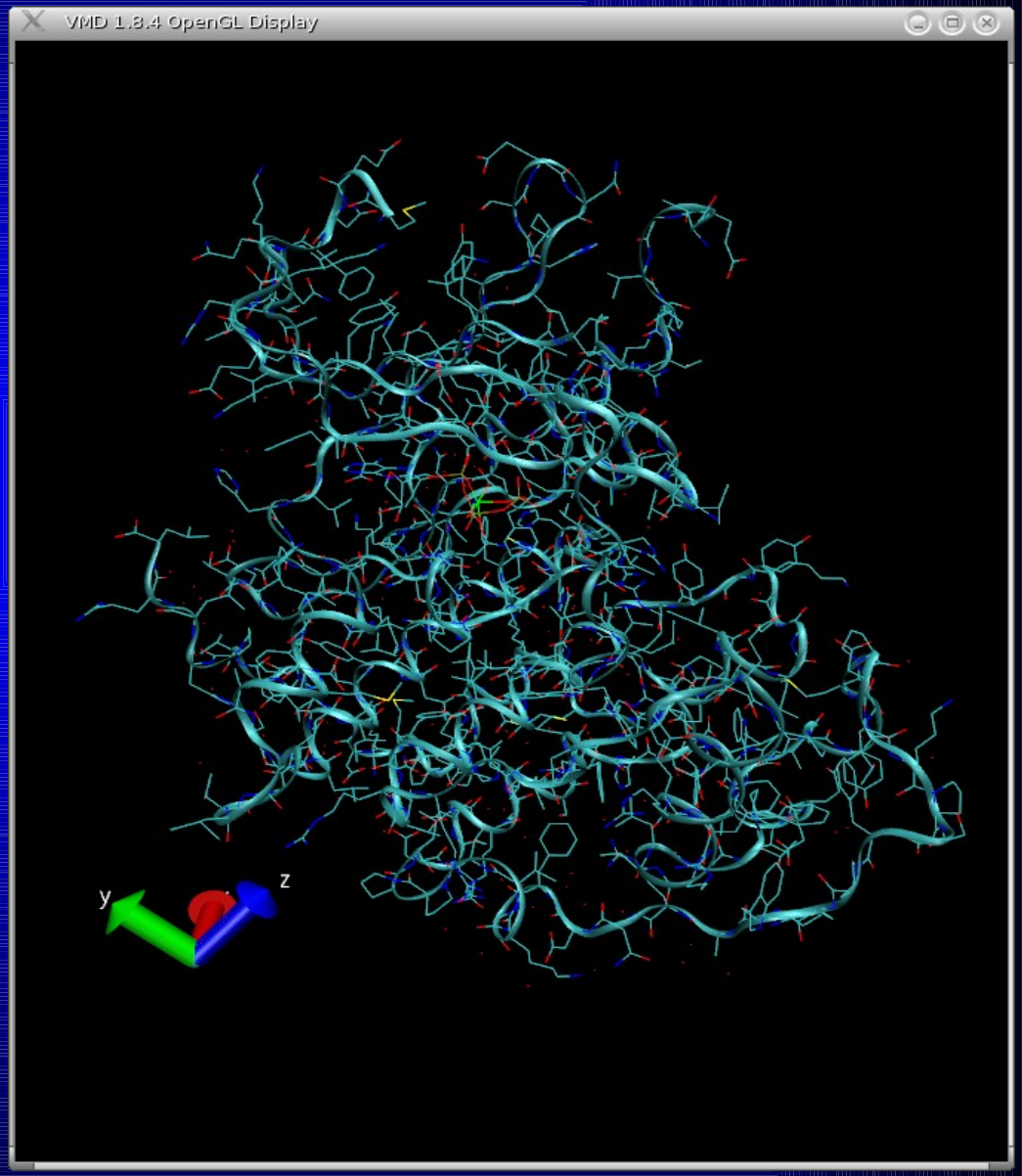
Zobrazení velkých molekul

CDK2 - 1hck.pdb

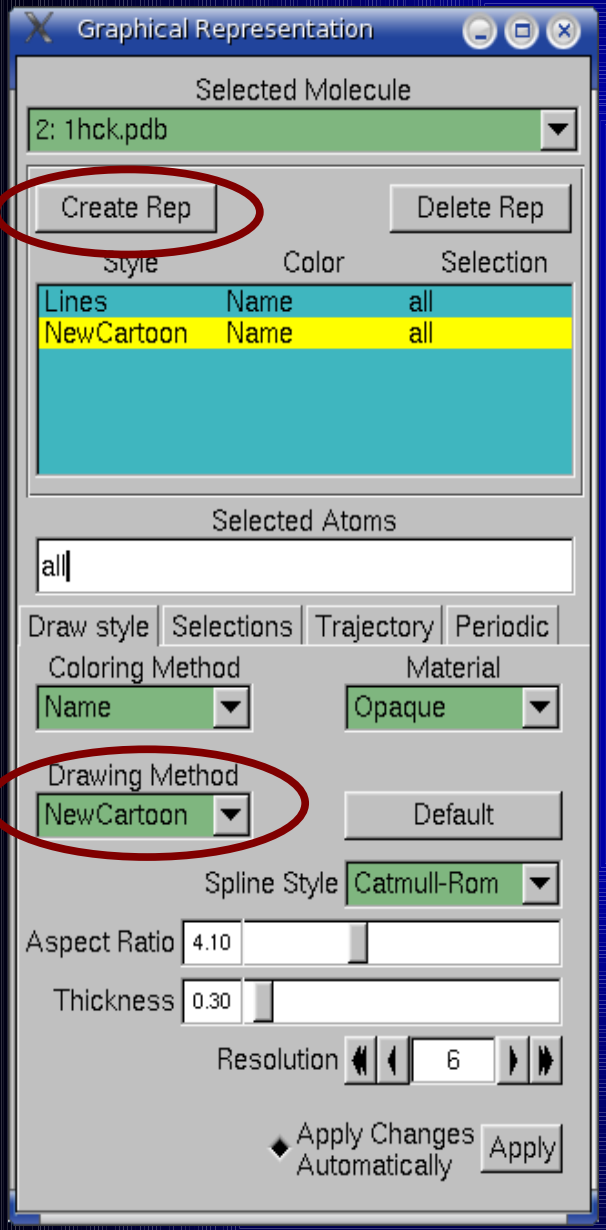


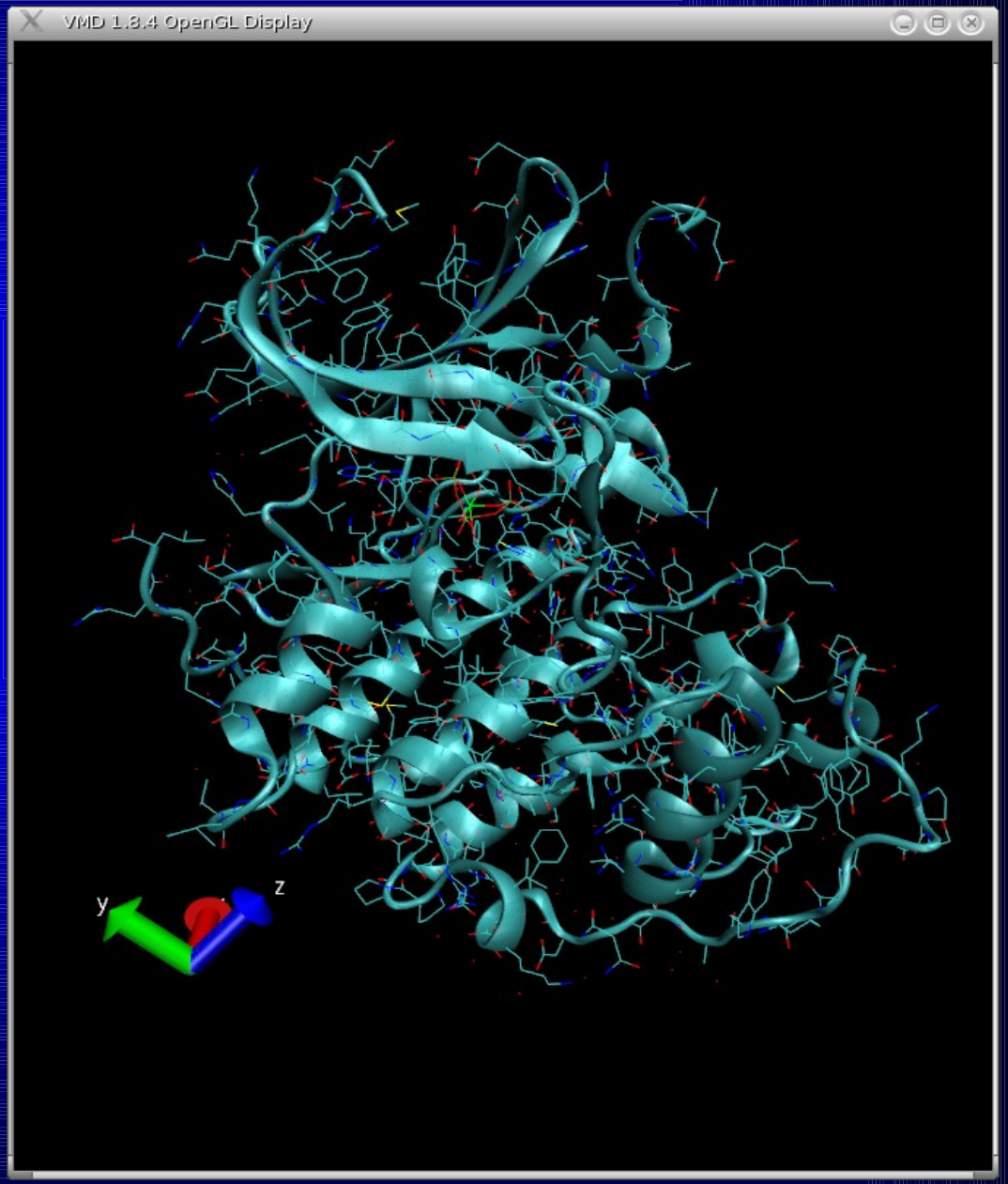
Zobrazení páteře proteinu



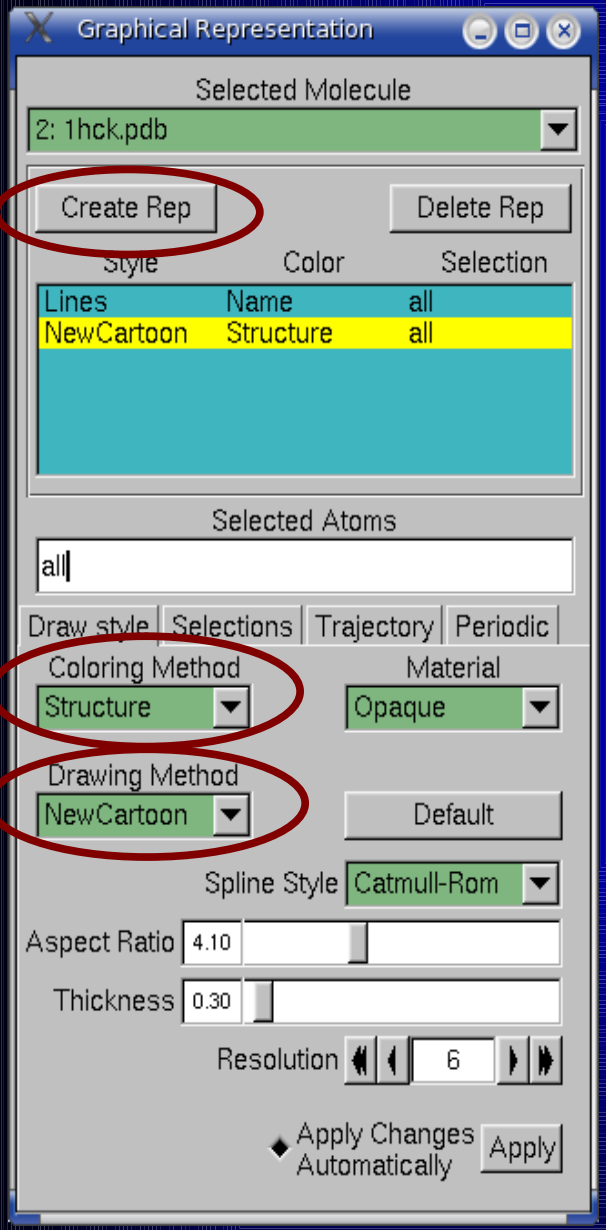


Zobrazení sekundární struktury proteinu

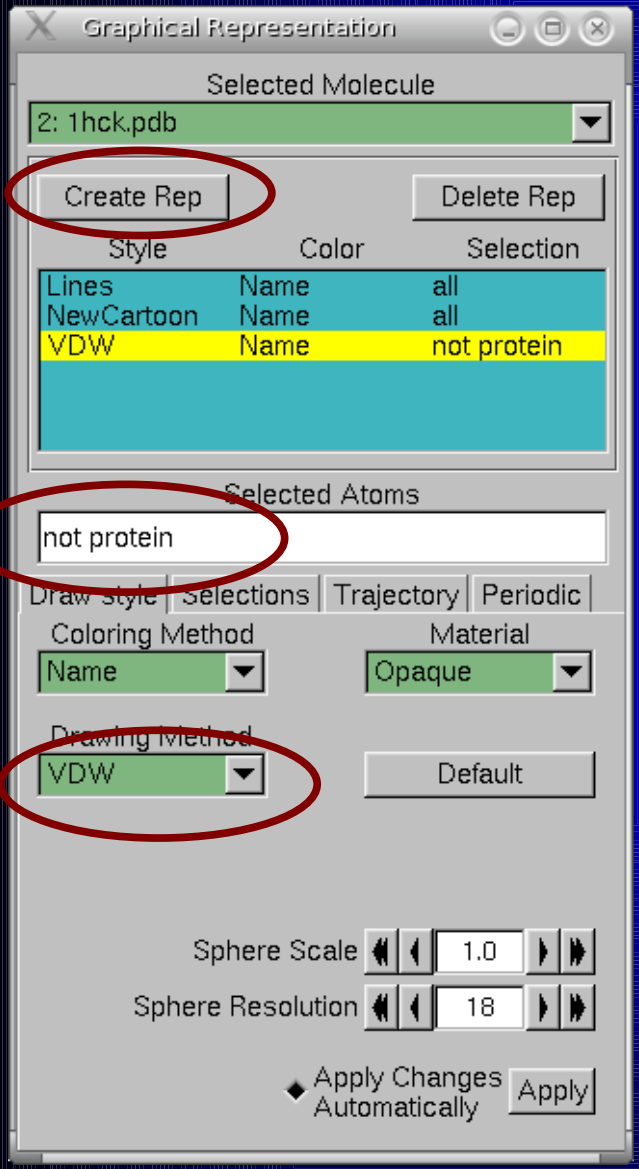


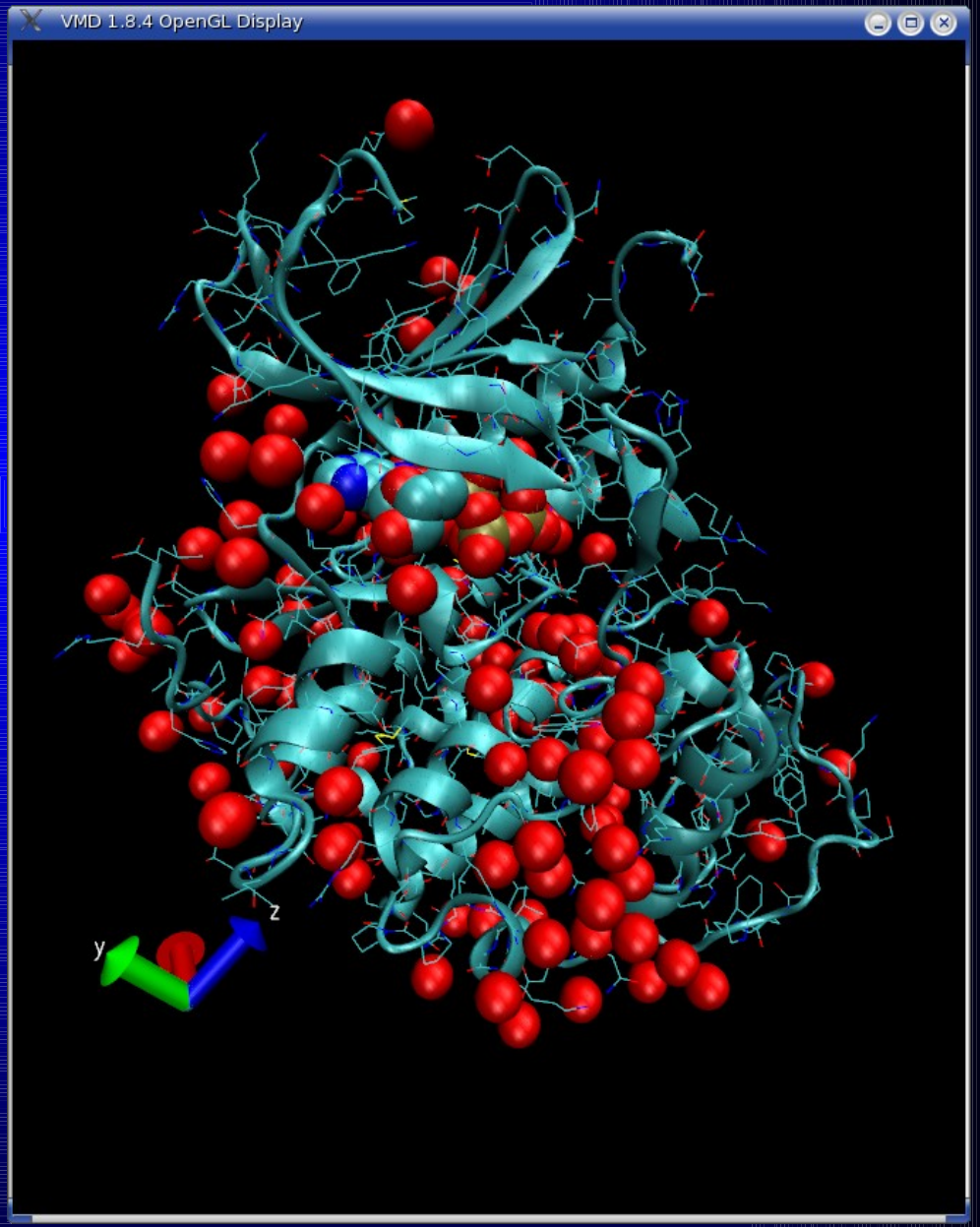


Zobrazení sekundární struktury proteinu

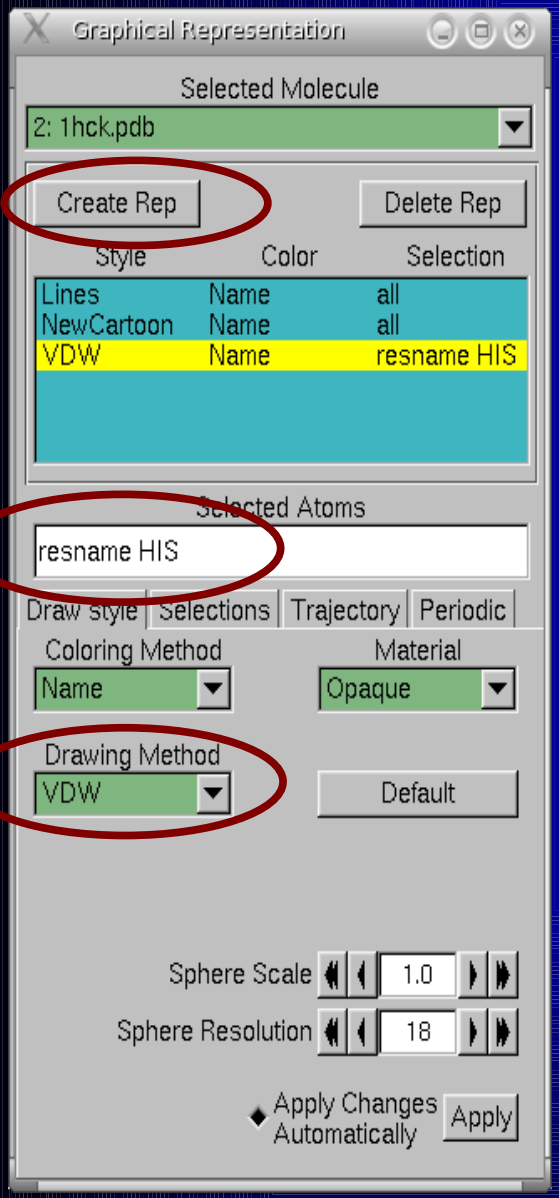


Zvýraznění neproteinových částí





Výběr určitých residuí proteinu



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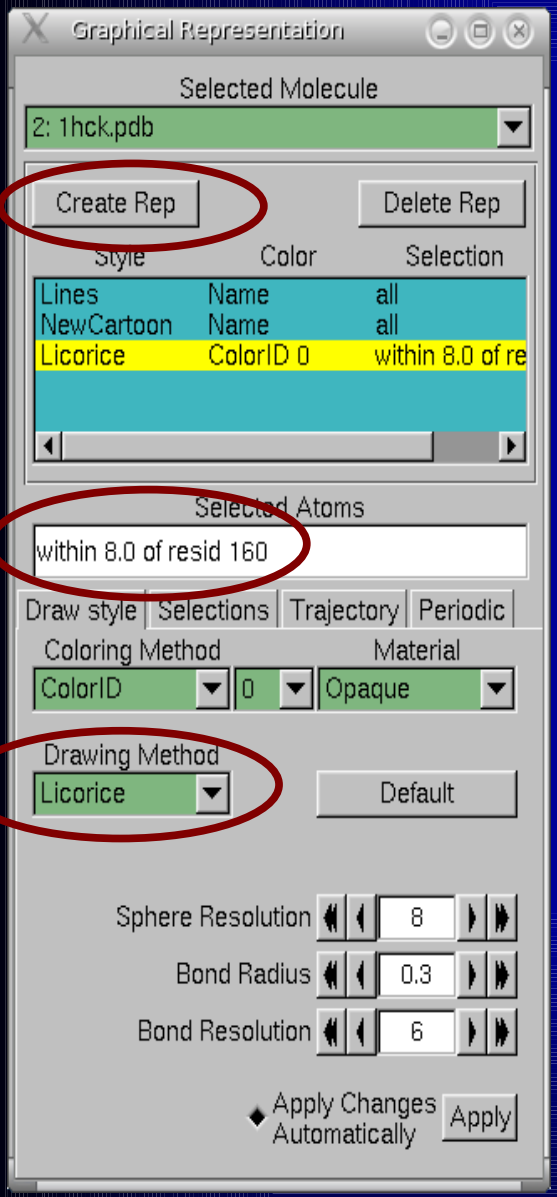
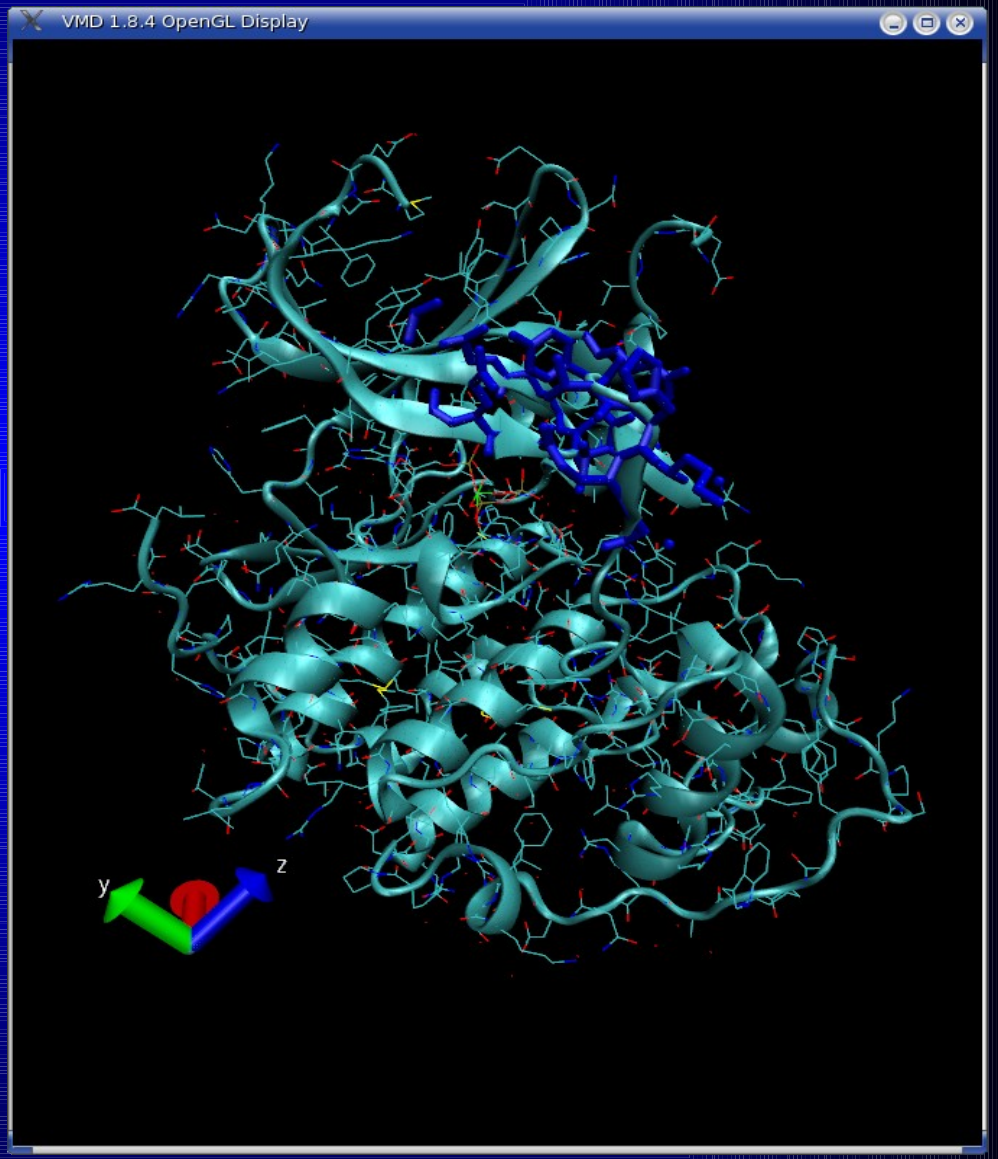
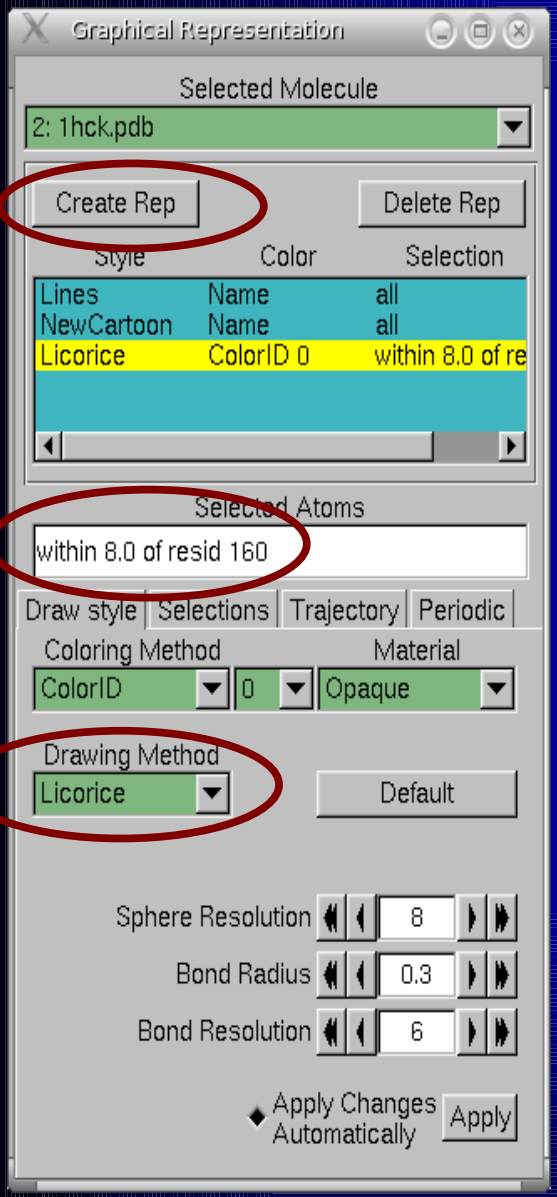
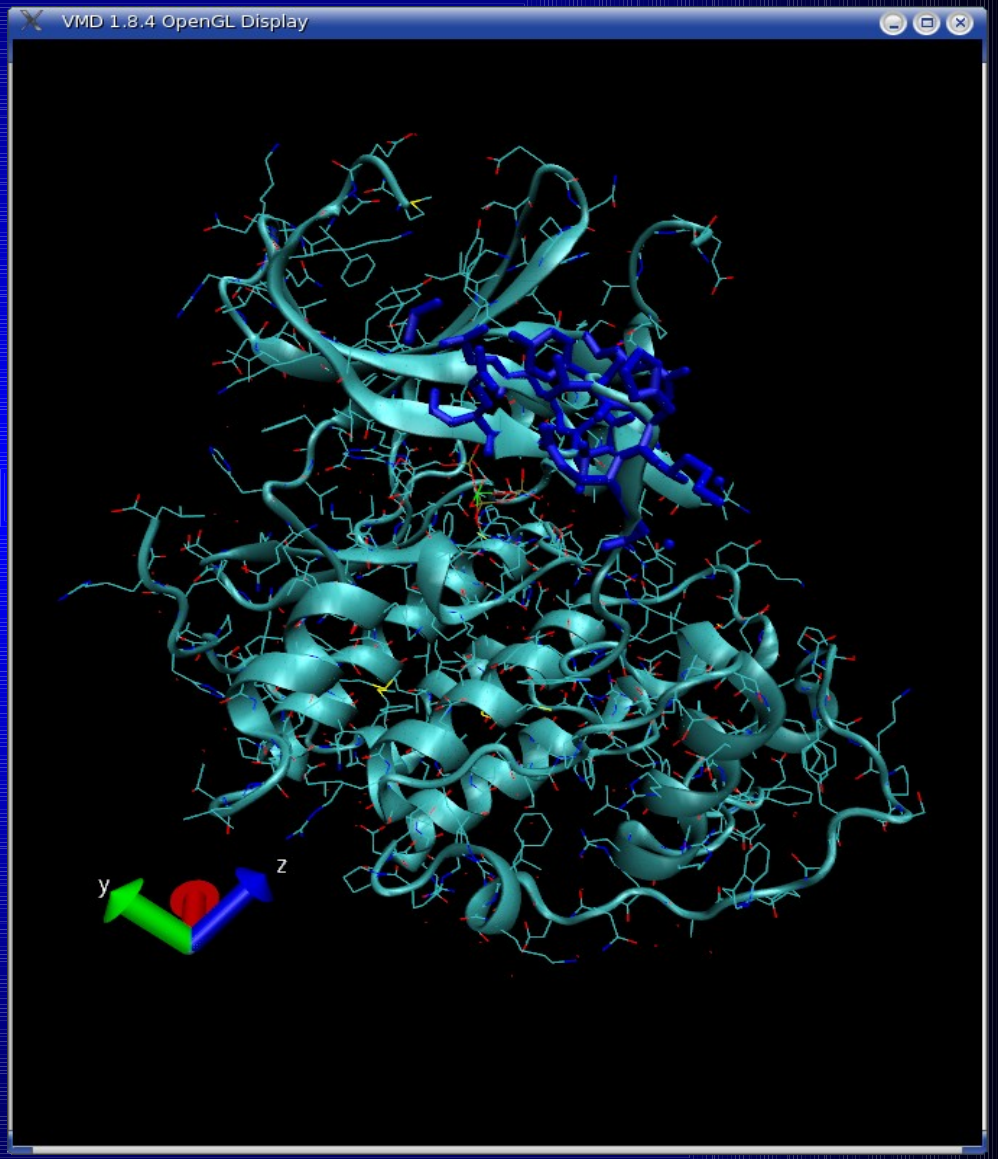


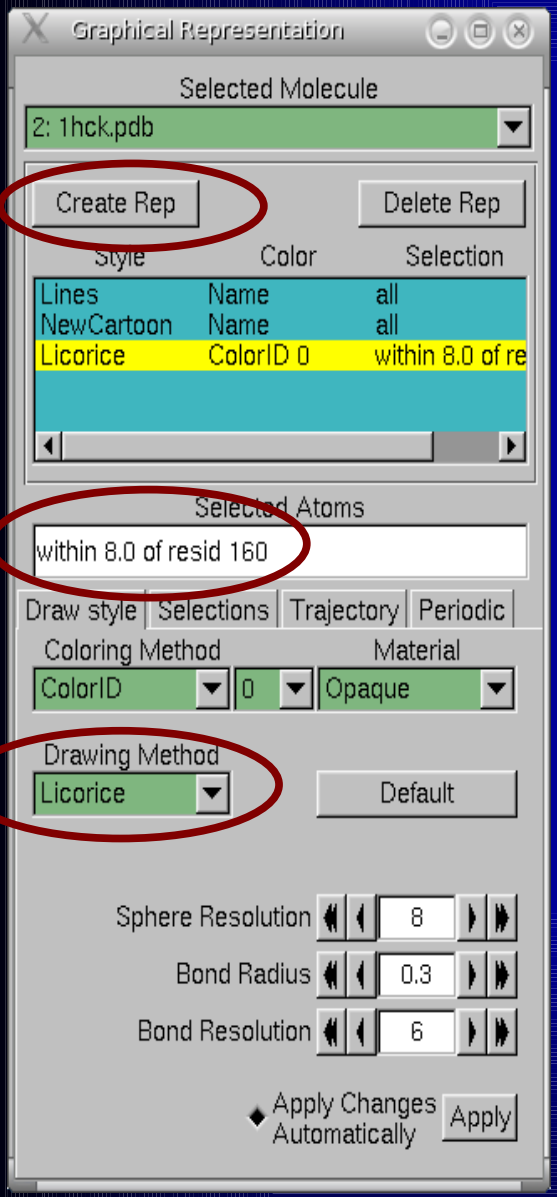


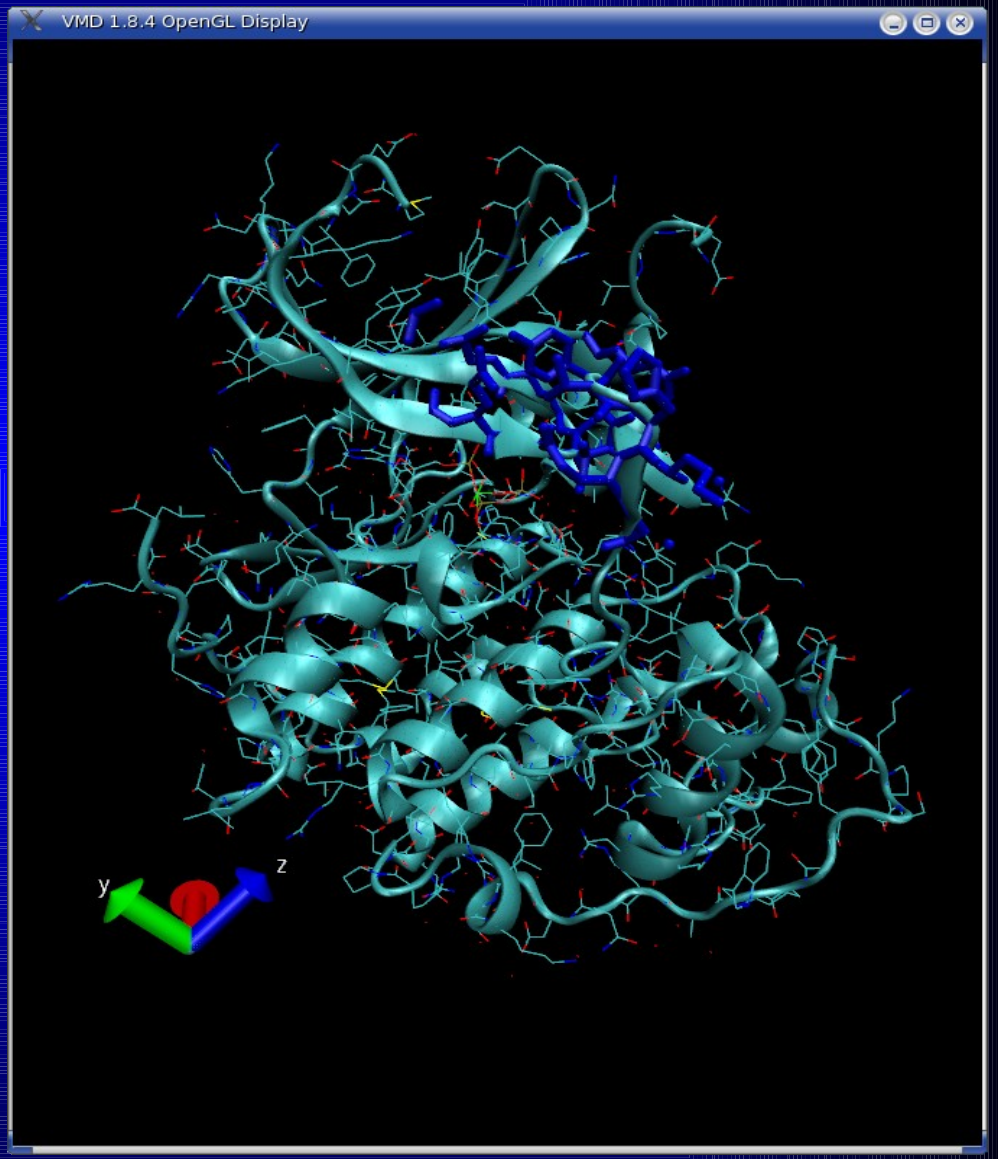
Výběr určitých residuí proteinu



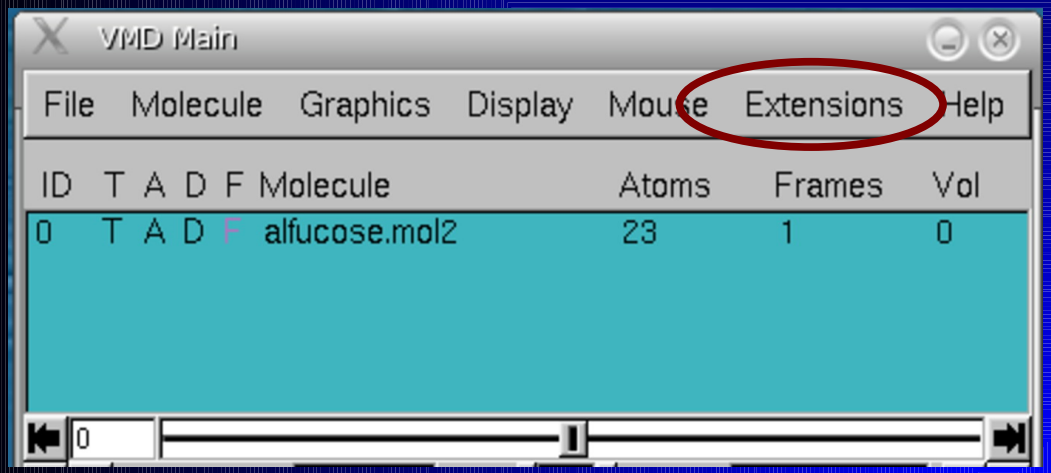


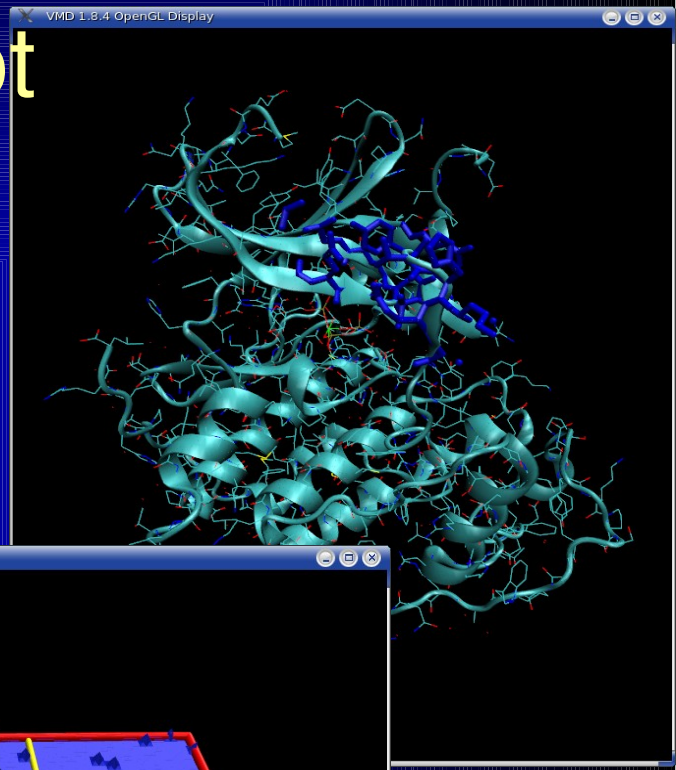
Výběr určitých residuí proteinu

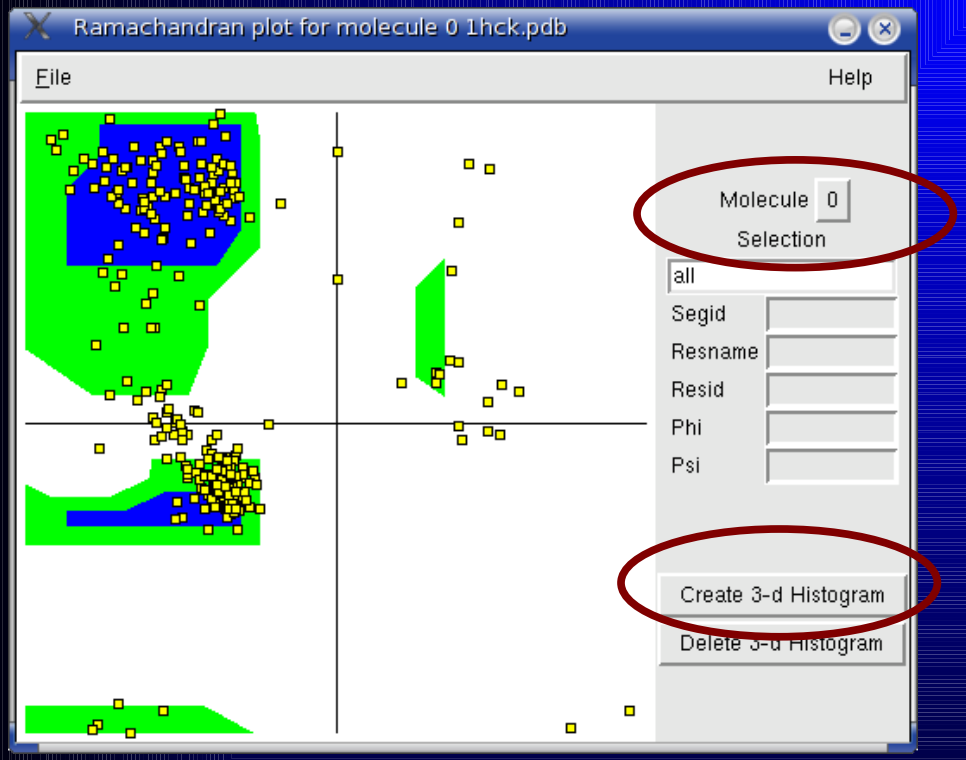


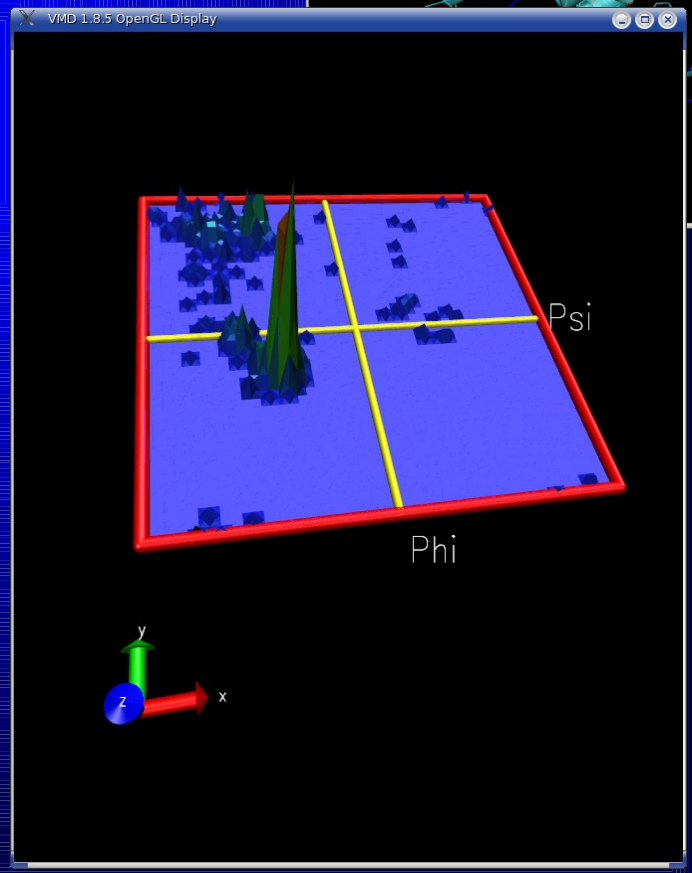


Ramachandran plot









Děkuji za pozornost ...