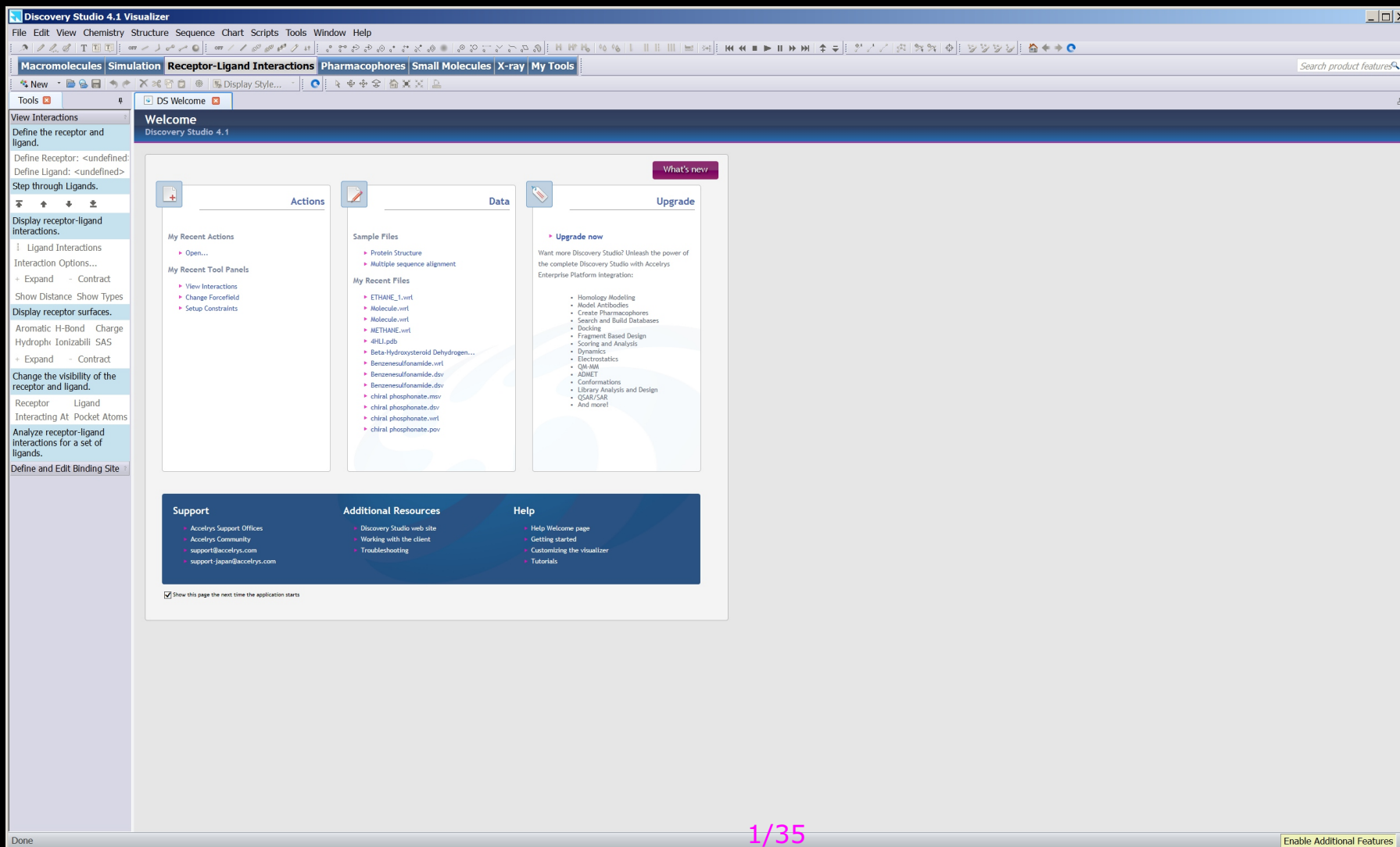


# UPUTSTVO ZA KORIŠĆENJE NEKIH FUNKCIJA PROGRAMA "DISCOVERY STUDIO 4.1 VISUALIZER"

Preuzeti i instalirati program "ds41clent.exe" koji je 64-bitni ili "ds41clent32bit.exe" koji je 32-bitni. Ukoliko je operativni sistem 64-bitni preporučuje se verzija "ds41clent.exe" mada i verzija "ds41clent32bit.exe" takođe treba da bude potpuno funkcionalna, ali znatno sporija. Ukoliko je operativni sistem 32-bitni moguće je instalirati samo verziju "ds41clent32bit.exe". Ove programe moguće je i direktno preuzeti sa sajta firme, posle besplatne registracije (<http://accelrys.com/products/discovery-studio/visualization-download.php>).

Posle instalacije, početni ekran izgleda kao što je prikazano:



U većini slučajeva, 3D strukture proteina, kompleksa protein-ligand kao i nukleinskih kiselina, određuju se rengenostrukturinom analizom. Tako se dobija, najčešće apsolutna i potpuna, konfiguracija molekula u tri dimenzije. Ovako određene strukture čuvaju se u obliku pogodnog 3D fajla, (pdb format i dr.), u onlajn databazama, odakle se mogu slobodno i neograničeno preuzimati. Posebno je značajna databaza PDB (Protein Data Bank), "<http://www.rcsb.org/pdb/home/home.do>". Takođe su, preko drugih onlajn databaza, dostupne i strukture velikog broja "malih molekula" tj. onih koji nisu biomakromolekuli.

Postoji veći broj besplatnih programa koji čitaju pdb fajlove i omogućavaju 3D rotaciju, translaciju, zumiranje, modifikovanje i dr. datog molekula. Međutim, za preciznu analizu molekula, kao i različite proračune, što je od posebnog značaja u razvoju novih lekova, najčešće se koriste komercijalni programi, mada postoje i oni koji su besplatni i slobodno dostupni.

Jedan od vodećih komercijalnih programa za sveobuhvatnu analizu, simulacije i proračune različitih parametara bio-makromolekula (ali i malih molekula) je Accelrys Discovery Studio, "<http://accelrys.com/products/discovery-studio/>", firme DASSAULT SYSTEMS, BIOVIA. Međutim, deo ovog programskog paketa, Accelrys DS Visualizer, slobodno je dostupan za nekomercijalnu primenu. Visualizer omogućava veoma raznovrsne operacije sa različitim 3D fajlovima, kao i direktnu konverziju pojedinih 2D fajlova (npr. Accelrys Draw skc formata) u približnu 3D strukturu. (Detaljan opis mogućnosti i komandi može se naći u Help fajlu Visualizer-a).

U nastavku ovog dokumenta, nalaze se neka osnovna uputstva za korišćenje Visualizer-a, u radu sa proteinima i kompleksima protein-ligand. Uputstva su prikazana u obliku "snimljenih ekrana" - *screen shots*. Sva navedena uputstva mogu se direktno primeniti i u radu sa malim molekulima. Program takođe sadrži i HELP fajl.

## PODEŠAVANJA PROGRAMA.

PROGRAM SE MOŽE PODEŠAVATI NA MNOGO RAZLIČITIH NAČINA. NEKA PODEŠAVANJA SU PRIKAZANA OVDE.

The image shows the Discovery Studio 4.1 Visualizer software interface. The main window displays a 'Welcome' screen with three columns: 'Actions', 'Data', and 'Upgrade now'. The 'Actions' column lists 'My Recent Actions' and 'My Recent Tool Panels'. The 'Data' column lists 'Sample Files' and 'My Recent Files'. The 'Upgrade now' section promotes the complete Discovery Studio Enterprise Platform integration.

A settings menu is open over the 'Upgrade now' section, listing various features with checkboxes:

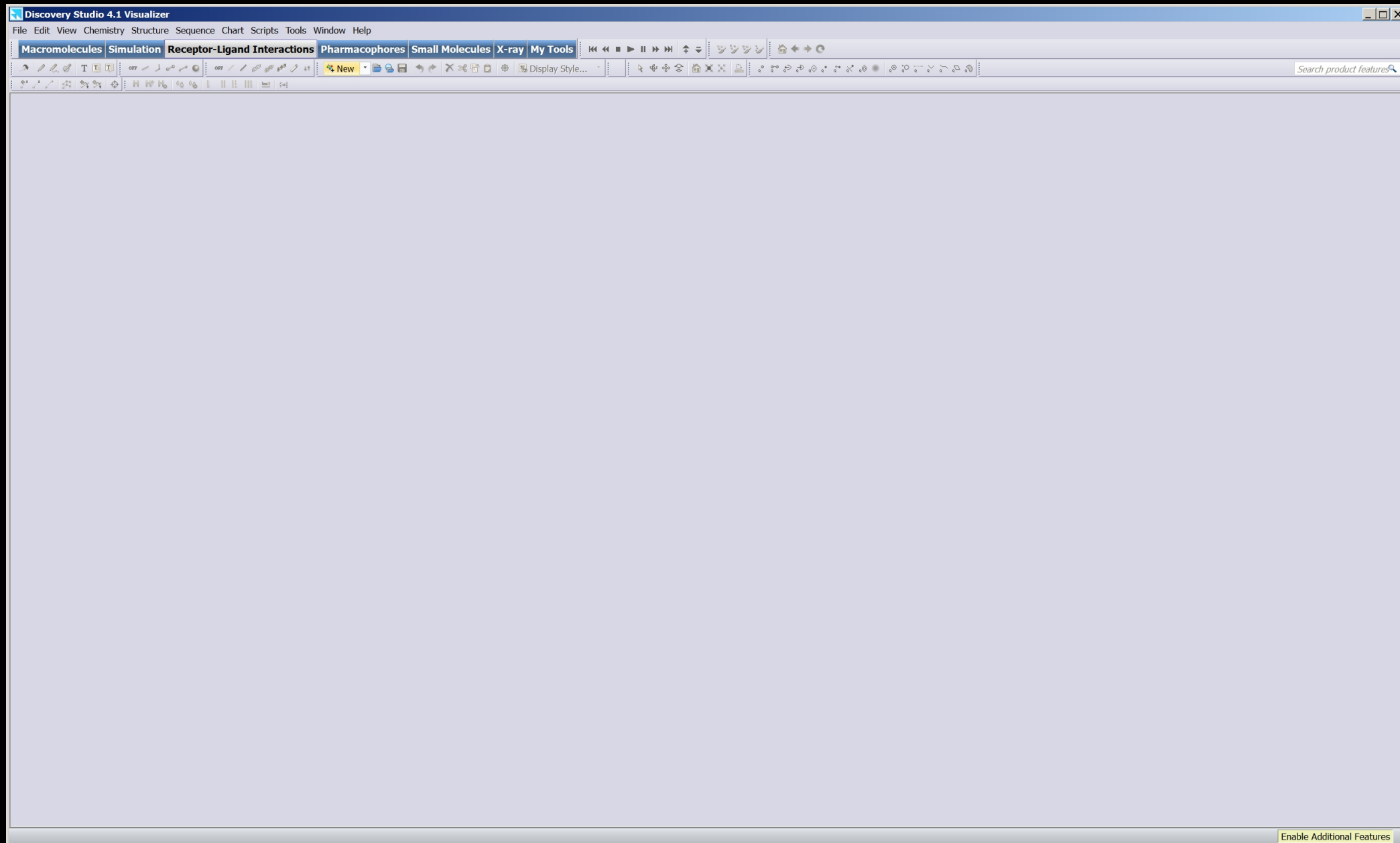
- Alignment
- Animation
- Atom Colors
- Atom Display
- Chemistry
- Search Product Features
- Navigation
- Nucleic Acid Structure Display
- Protein Structure Display
- Query
- Scripting
- Sequence
- Sketching
- Smart Tools
- Standard
- View

The left sidebar contains several tool panels:

- View Interactions**: Define the receptor and ligand, Define Receptor, Define Ligand, Step through Ligands, Display receptor-ligand interactions, Ligand Interactions, Interaction Options, Show Distance, Show Types, Display receptor surfaces, Aromatic H-Bond, Charge, Hydrophobic, Ionizable, SAS, Change the visibility of the receptor and ligand, Receptor, Ligand, Interacting At, Pocket Atoms, Analyze receptor-ligand interactions for a set of ligands, Define and Edit Binding Site.

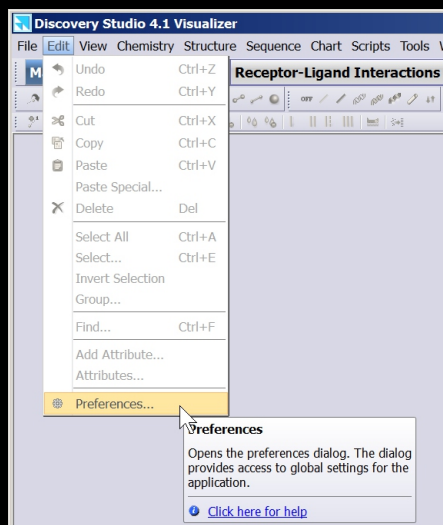
At the bottom right, there is a button labeled 'Enable Additional Features'.

PODEŠAVANJA PROGRAMA.  
IZGLED EKRANA POSLE PODEŠAVANJA SA PRETHODNE STRANE.

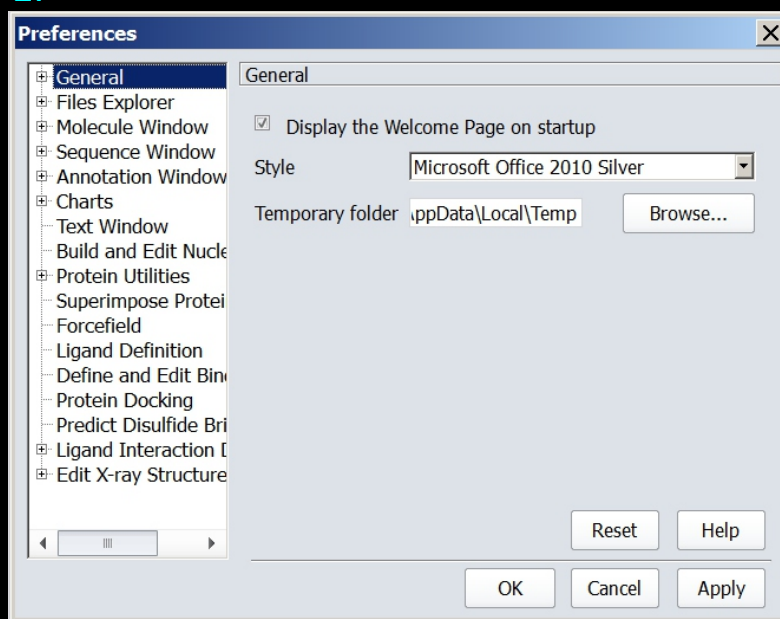


# PODEŠAVANJA PROGRAMA. DALJA PODEŠAVANJA.

1.

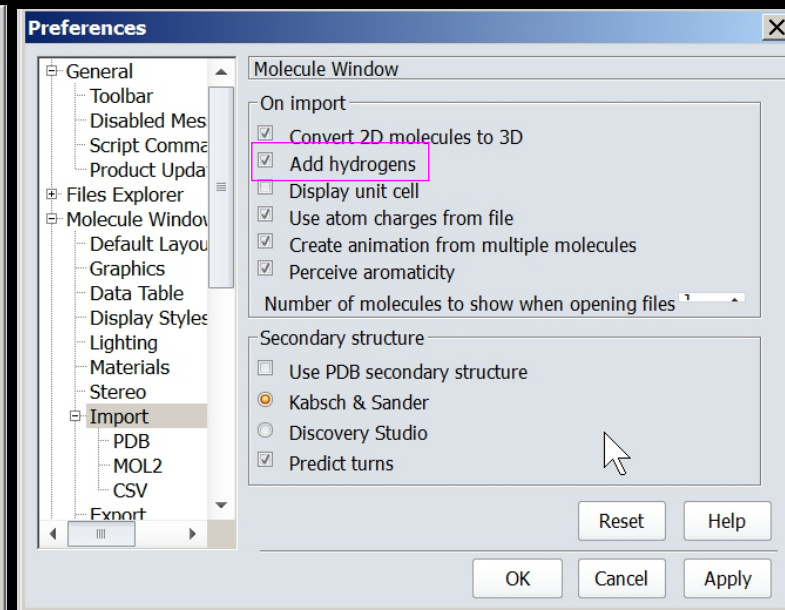


2.

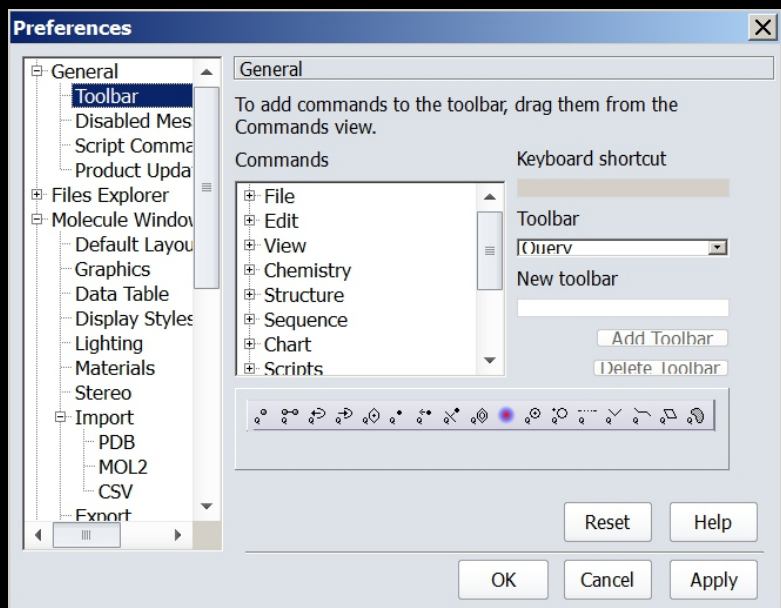


3.

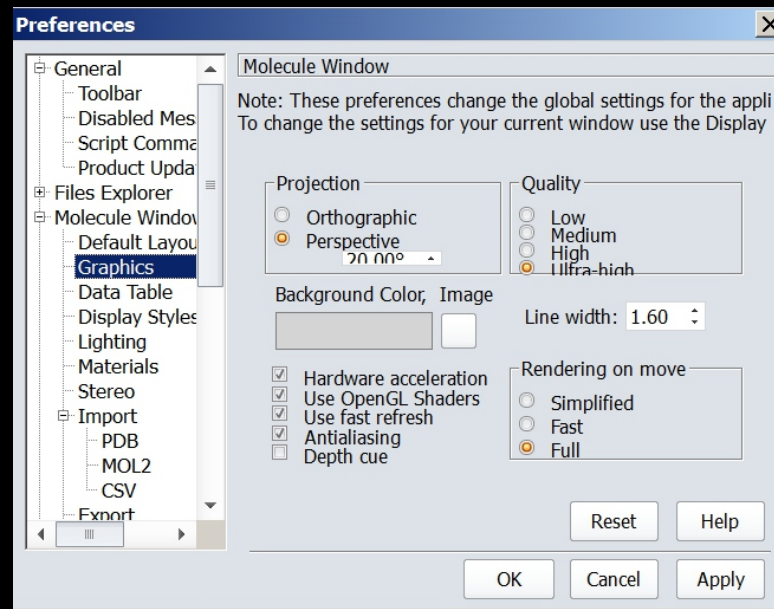
OBRATITI PAŽNJU DA JE OPCIJA  
"Add hydrogens" UKLJUČENA



4.



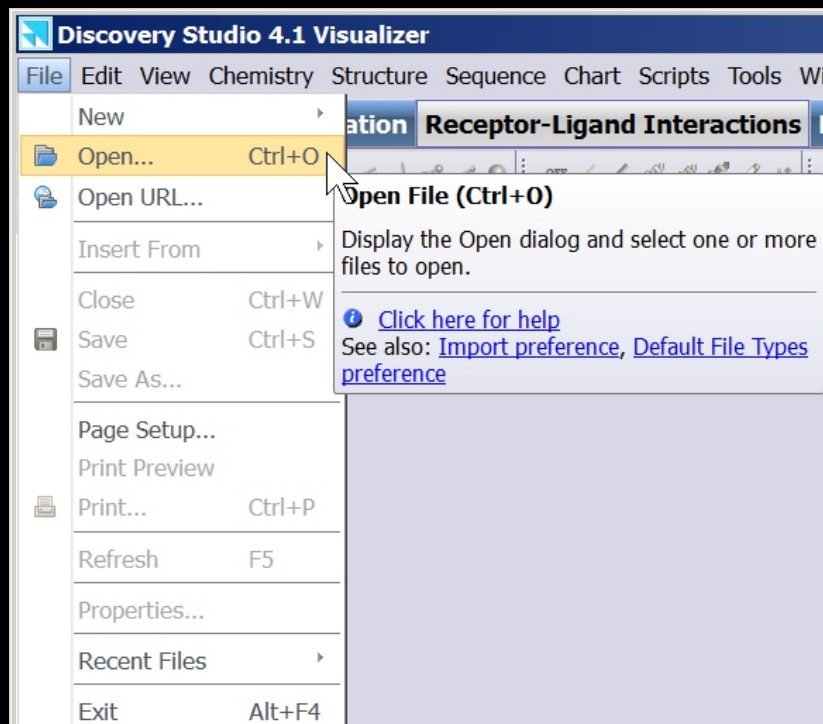
5.



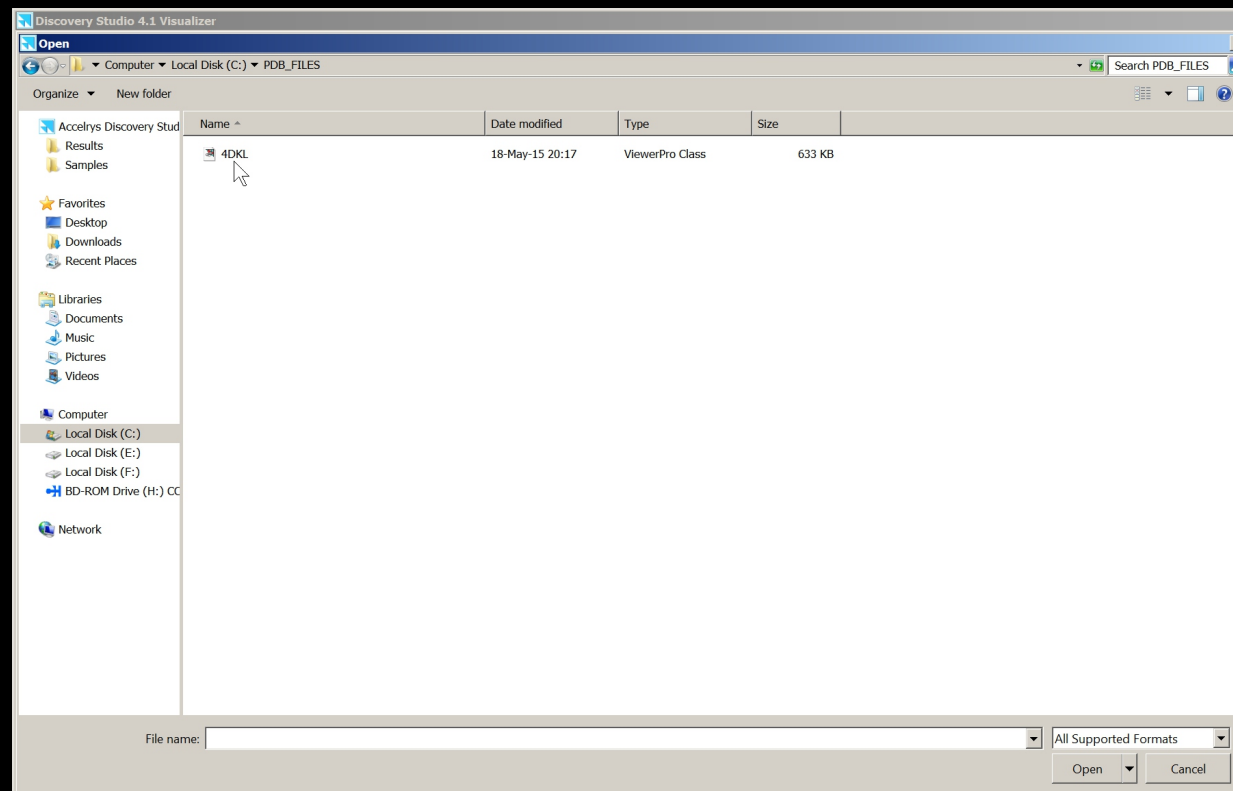
NAPOMENA.  
VREDNOSTI POD  
5. PODEŠTI PREMA  
HARDVERSKIM  
MOGUĆNOSTIMA  
RAČUNARA, A  
POSEBNO  
"Quality".  
(Vrednost "Ultra  
high" može  
potpuno da blokira  
hardverski slabije  
računare)

# ZATIM OTVORITI PREUZETI PDB FAJL (PRIMER 4DKL).

1.

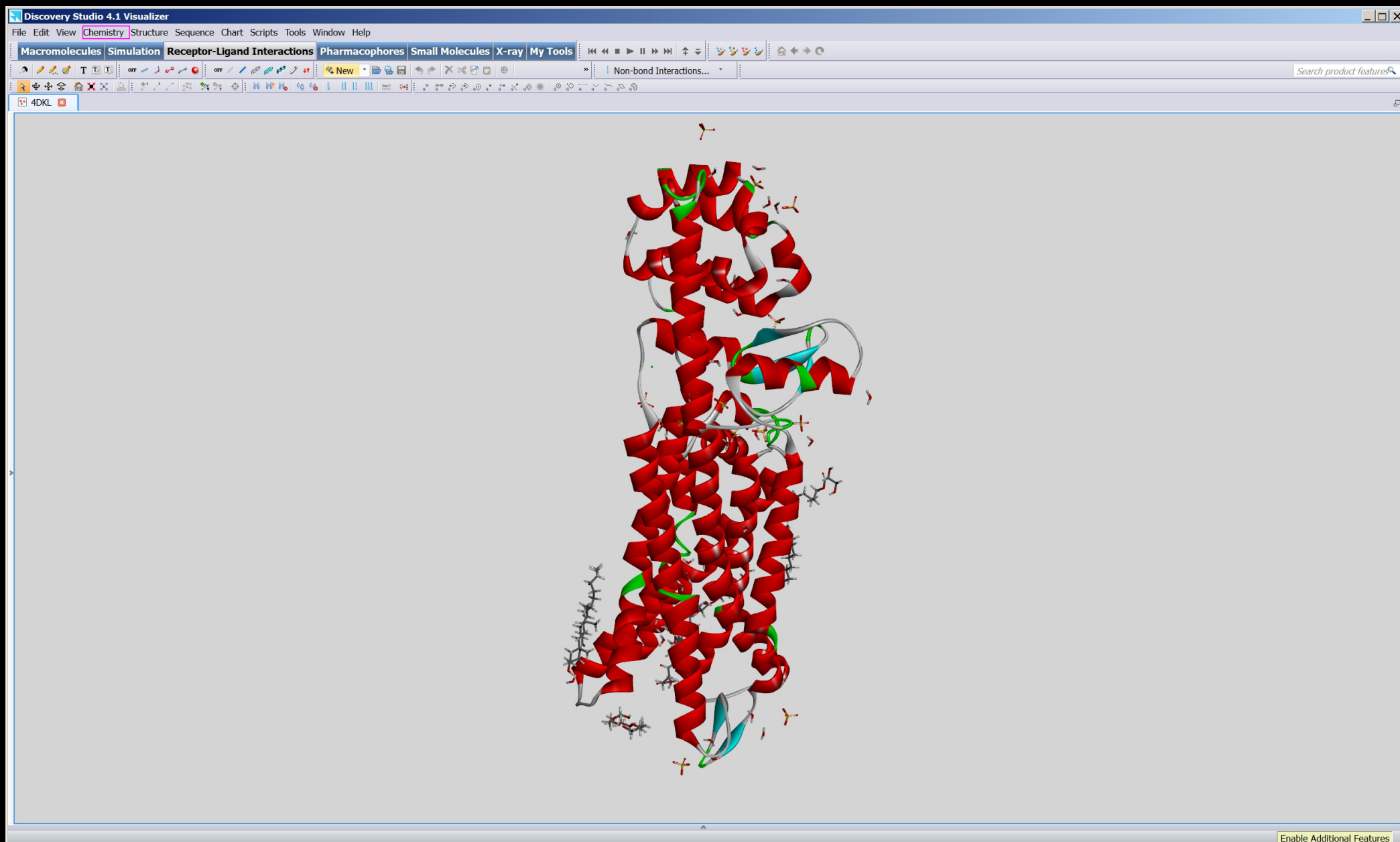


2.



POČETNI IZGLED EKRANA POSLE OTVARANJA FAJLA.

Ukoliko nedostaju H atomi, dodati ih preko menija: Chemistry/Hydrogens/Add



# ISPROBATI RAZLIČITE MOGUĆNOSTI PRIKAZIVANJA MOLEKULA KAO ŠTO JE PRIKAZANO NA SLEDEĆIM SLIKAMA.

The image shows the Discovery Studio 4.1 Visualizer interface. The main window displays a protein structure (4DKL) rendered as a red ribbon. A context menu is open over the protein, with the 'Display Style...' option selected. A tooltip for 'Display Style (Ctrl+D)' explains that it changes the display style of the selected item(s). Two 'Display Style' dialog boxes are overlaid on the right side of the interface. The top dialog, labeled '2.', is for the 'Atom' tab, showing options for 'Display style' (Line is selected) and 'Coloring' (Color by: Element). The bottom dialog, labeled '3.', is for the 'Protein' tab, showing options for 'Display style' (Solid ribbon is selected) and 'Coloring' (Color by: Secondary Type). Both dialogs include 'OK', 'Cancel', 'Apply', and 'Help' buttons.

**1.** PRITISNUTI DESNO DUGME MIŠA

**2.** Display Style

Atom Protein Cell Graphics Lighting Materials

Display style

Off

Line

Stick

Ball and stick

Scaled ball and stick

CPK

Polyhedron

Coloring

Color by:

Element

Colors...

Custom:

Carbon atoms only

Show bond order

Ball size: 0.40 Stick size: 0.20 CPK scale: 1.00

OK Cancel Apply Help

**3.** Display Style

Atom Protein Cell Graphics Lighting Materials

Display style

Off

Ca wire

Ca stick

Line ribbon

Flat ribbon

Solid ribbon

Tube

Schematic

Coloring

Color by:

Secondary Type

Colors...

Custom:

Ribbon size

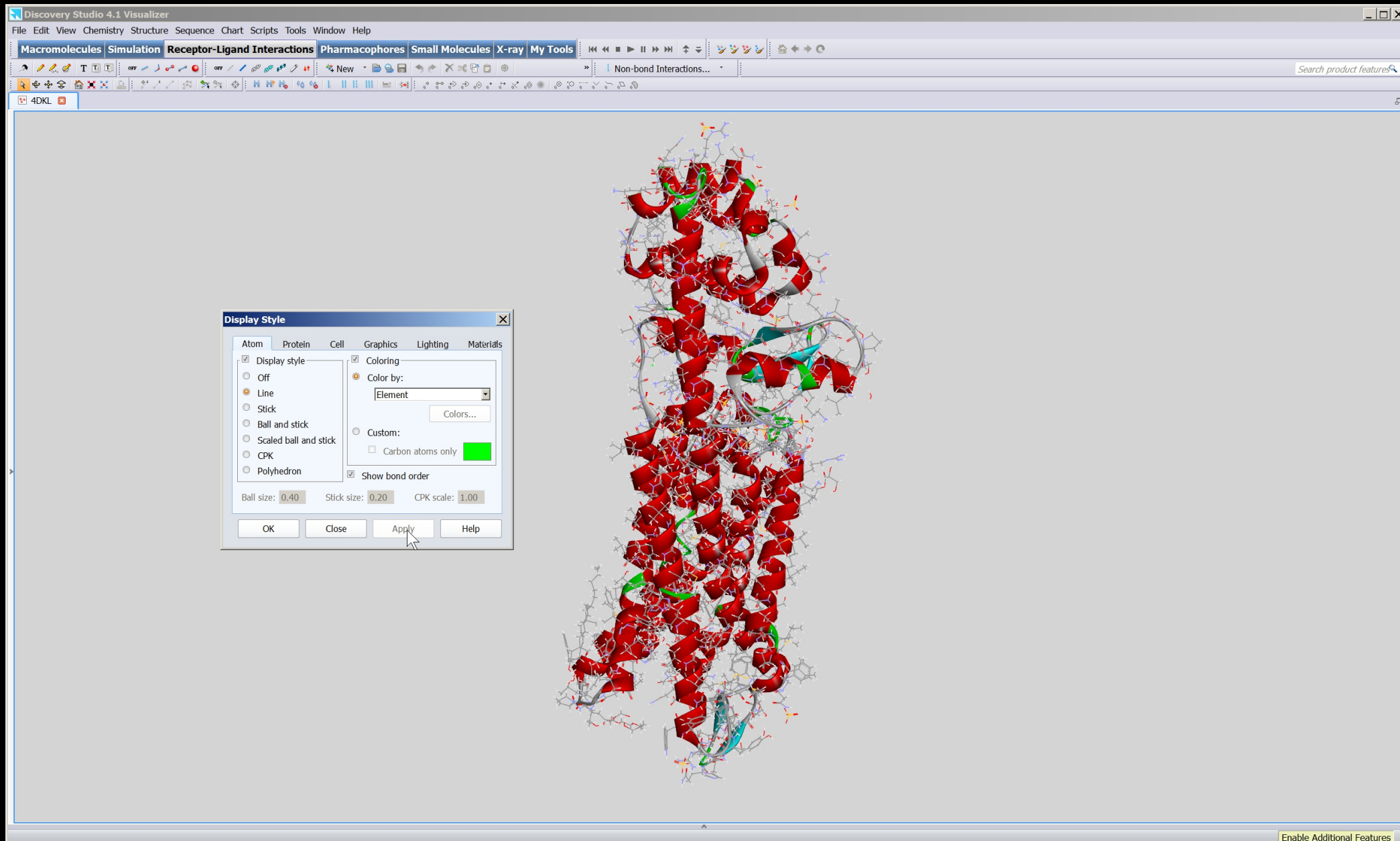
Default Ribbon Size

Display size: 1.00

OK Cancel Apply Help



# ISPROBATI RAZLIČITE MOGUĆNOSTI PRIKAZIVANJA MOLEKULA KAO ŠTO JE PRIKAZANO NA SLEDEĆIM SLIKAMA.



# ISPROBATI RAZLIČITE MOGUĆNOSTI PRIKAZIVANJA MOLEKULA KAO ŠTO JE PRIKAZANO NA SLEDEĆIM SLIKAMA.

The image shows a screenshot of the Discovery Studio 4.1 Visualizer software interface. The main window displays a 3D molecular model of a protein-ligand complex. The protein is shown as a red surface, and the ligand is shown as a stick model with a cyan and green color scheme. A 'Display Style' dialog box is open in the foreground, showing the 'Graphics' tab. The dialog box has several options for visualization:

- Projection:** Orthographic (unselected), Perspective (selected), 20.00° (angle)
- Quality:** Low (unselected), Medium (unselected), High (unselected), Ultra-high (selected)
- Background Color, Image:** A black color swatch and an image icon.
- Line width:** 1.60
- Depth cue:** Unchecked checkbox

Buttons at the bottom of the dialog box are OK, Close, Apply, and Help. The software interface includes a menu bar (File, Edit, View, Chemistry, Structure, Sequence, Chart, Scripts, Tools, Window, Help) and a toolbar with various icons for file operations and visualization. The title bar reads 'Discovery Studio 4.1 Visualizer' and the window name is '4DKL'. A search bar at the top right contains the text 'Search product features'. A status bar at the bottom right says 'Enable Additional Features'.

ISPROBATI RAZLIČITE MOGUĆNOSTI PRIKAZIVANJA MOLEKULA KAO ŠTO JE PRIKAZANO NA SLEDEĆIM SLIKAMA.

The image shows the Discovery Studio 4.1 Visualizer interface. The main window displays a 3D model of a protein-ligand complex. The protein is shown as a red surface with a white ribbon backbone. The ligand is shown as a stick model with red, green, and blue atoms. Two 'Display Style' dialog boxes are open, demonstrating different rendering options.

The left dialog box is titled 'Display Style' and has tabs for Atom, Protein, Cell, Graphics, Lighting, and Materials. The 'Lighting' tab is selected. It shows a preview of a sphere with four numbered lights (1, 2, 3, 4) and checkboxes for 'Light 1', 'Light 2', 'Light 3', and 'Light 4'. Below the preview are sliders for 'Ambient Shadow' and 'Direct Shadow', and checkboxes for 'Depth Blur' and 'Atom Outline'. The 'Apply' button is highlighted.

The right dialog box is also titled 'Display Style' and has tabs for Protein, Cell, Graphics, Lighting, and Materials. The 'Materials' tab is selected. It shows a preview of a sphere with three colored atoms (red, green, blue) and sliders for 'Ambient', 'Diffuse', 'Specular', 'Emission', and 'Shininess'. Below the preview are buttons for 'Chalk', 'Metallic', 'Plastic', and 'Rubber'. The 'Apply' button is highlighted.

# ISPROBATI RAZLIČITE MOGUĆNOSTI PRIKAZIVANJA MOLEKULA KAO ŠTO JE PRIKAZANO NA SLEDEĆIM SLIKAMA.

The image shows a screenshot of the Discovery Studio 4.1 Visualizer software interface. The main window displays a 3D ribbon representation of a protein structure, colored by secondary type (red, green, blue, and white). The protein is shown in a ribbon representation, with atoms represented as small spheres. The interface includes a menu bar (File, Edit, View, Chemistry, Structure, Sequence, Chart, Scripts, Tools, Window, Help) and a toolbar with various icons for editing and visualization. A 'Display Style' dialog box is open in the foreground, showing options for displaying the protein structure. The dialog box has tabs for Atom, Protein, Cell, Graphics, Lighting, and Materials. The 'Protein' tab is selected, and the 'Display style' section is checked. The 'Coloring' section is also checked, with 'Color by:' set to 'Secondary Type'. The 'Ribbon size' section is checked, with 'Default Ribbon Size' selected. The 'Display size' is set to 1.00. The dialog box has buttons for OK, Close, Apply, and Help.

Discovery Studio 4.1 Visualizer

File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help

Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools

Non-bond Interactions... Search product features

4DKL

Display Style

Atom Protein Cell Graphics Lighting Materials

Display style

Off

Ca wire

Ca stick

Line ribbon

Flat ribbon

Solid ribbon

Tube

Schematic

Display size: 1.00

Coloring

Color by:

Secondary Type

Colors...

Custom:

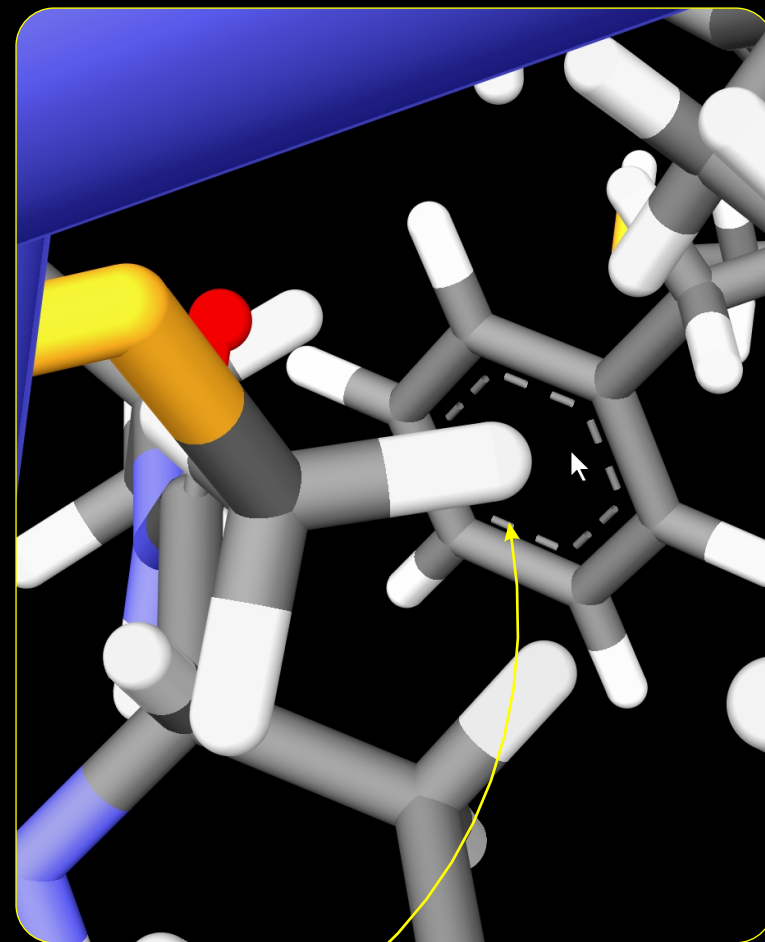
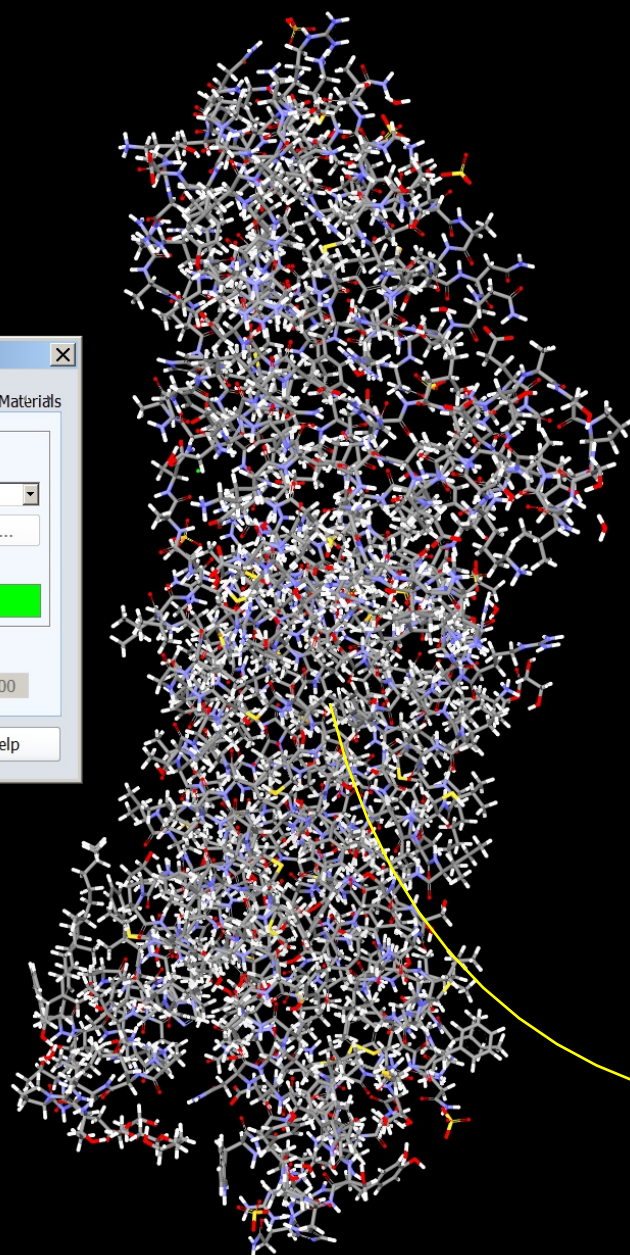
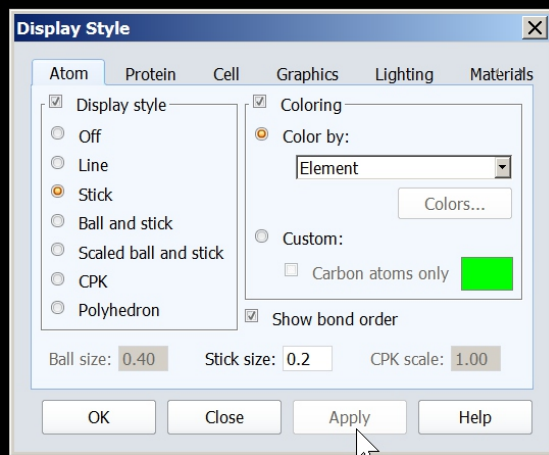
Ribbon size

Default Ribbon Size

OK Close Apply Help

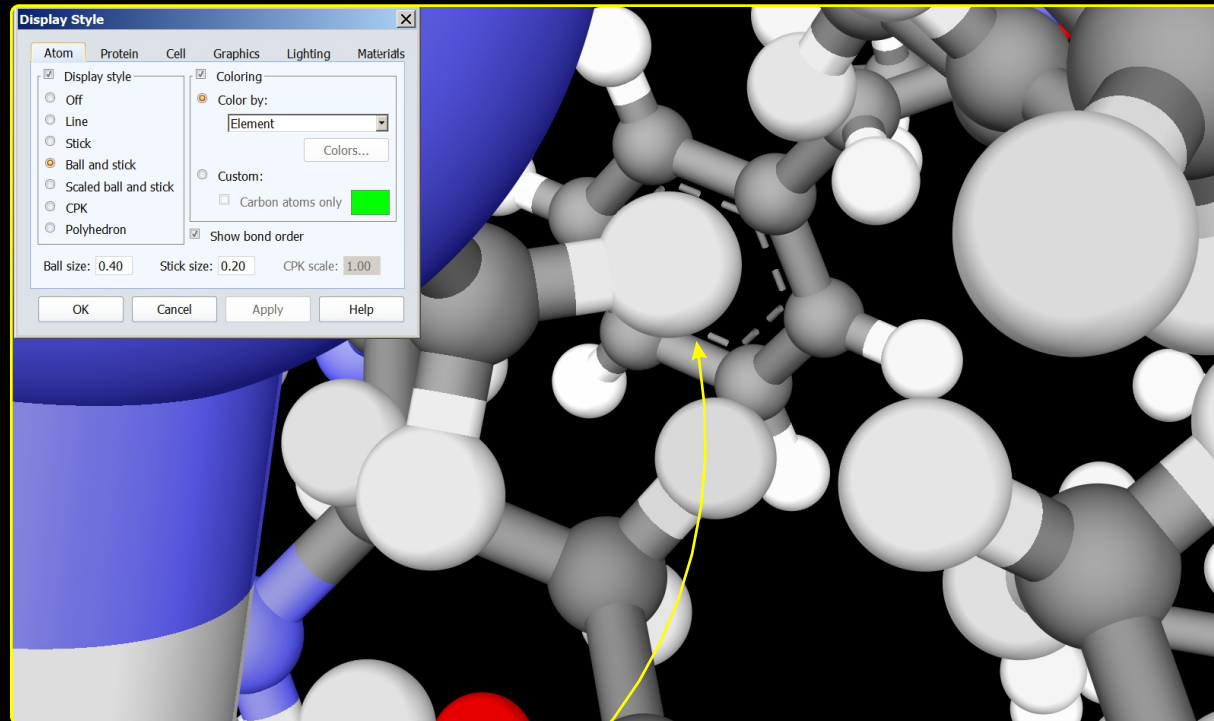
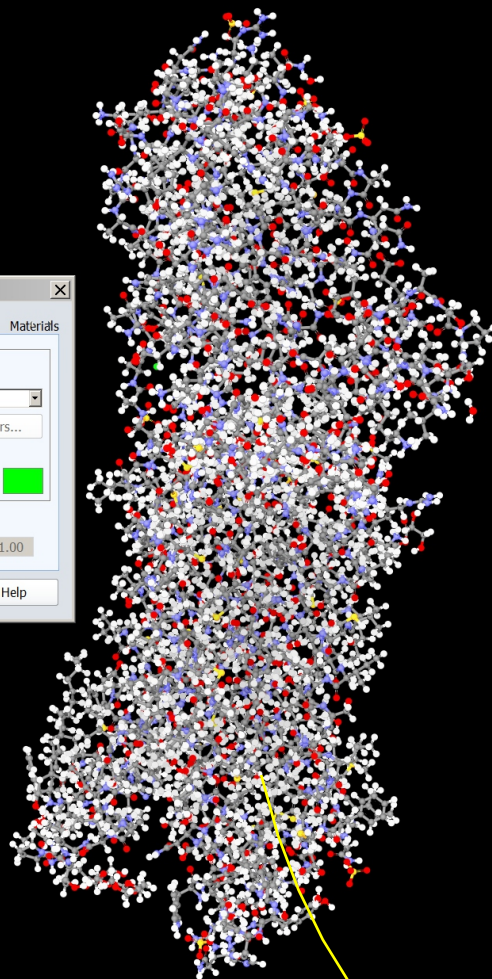
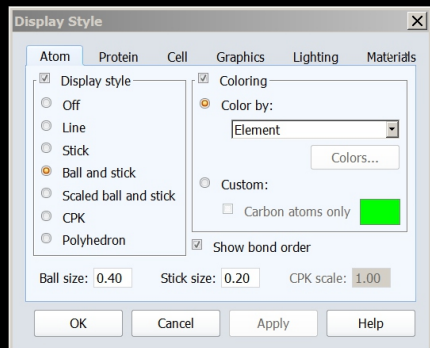
Enable Additional Features

ISPROBATI RAZLIČITE MOGUĆNOSTI PRIKAZIVANJA MOLEKULA KAO ŠTO JE PRIKAZANO NA SLEDEĆIM SLIKAMA.



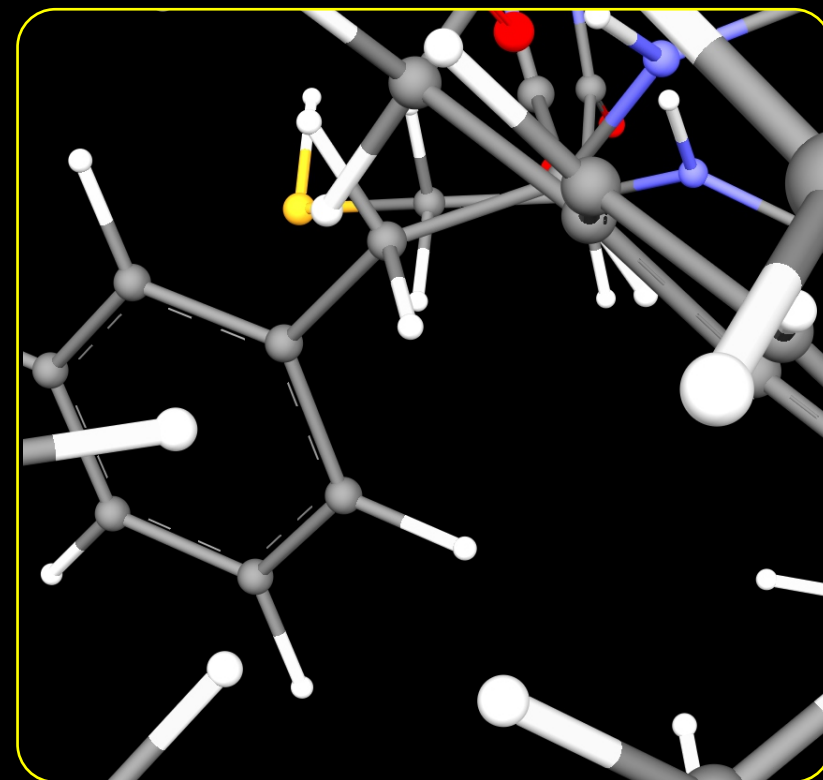
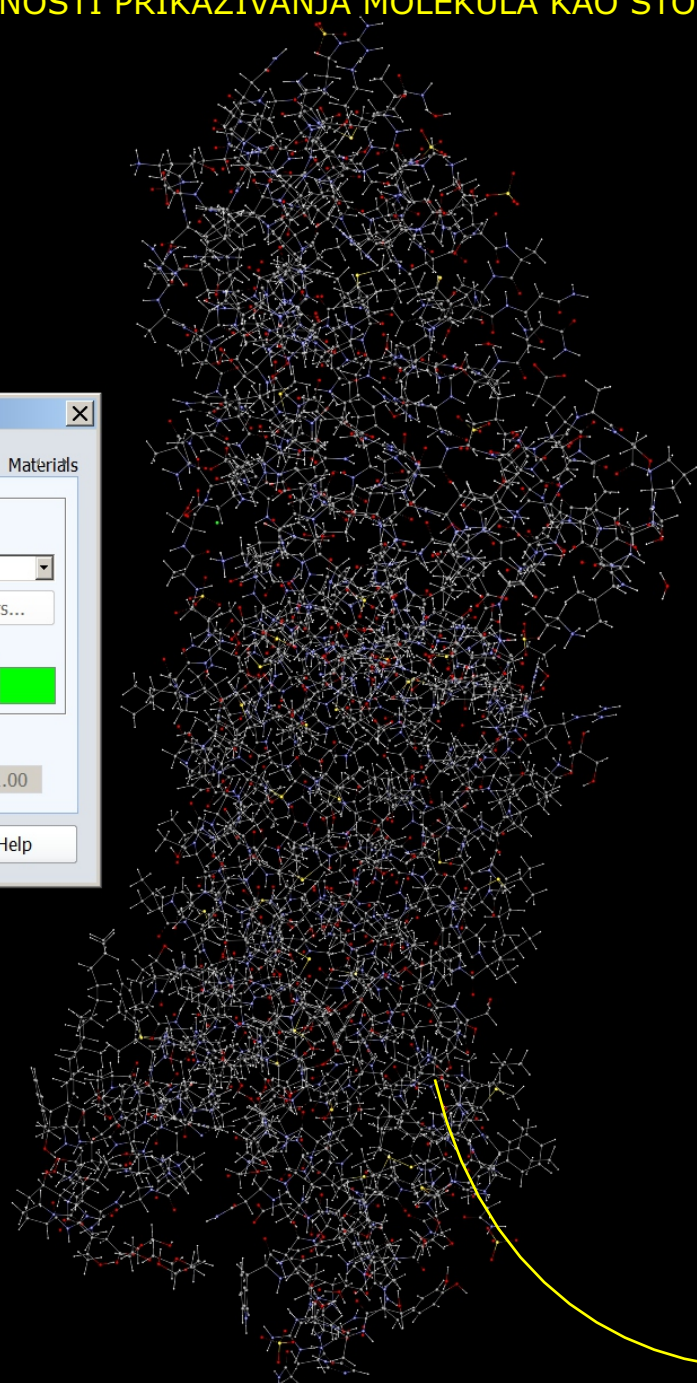
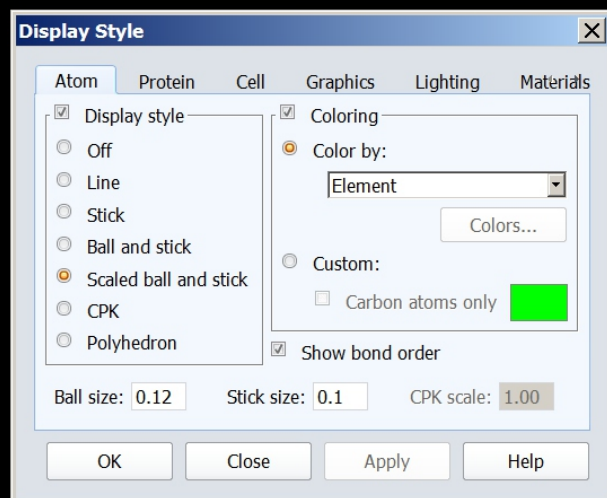
UVEĆANA SLIKA

ISPROBATI RAZLIČITE MOGUĆNOSTI PRIKAZIVANJA MOLEKULA KAO ŠTO JE PRIKAZANO NA SLEDEĆIM SLIKAMA.



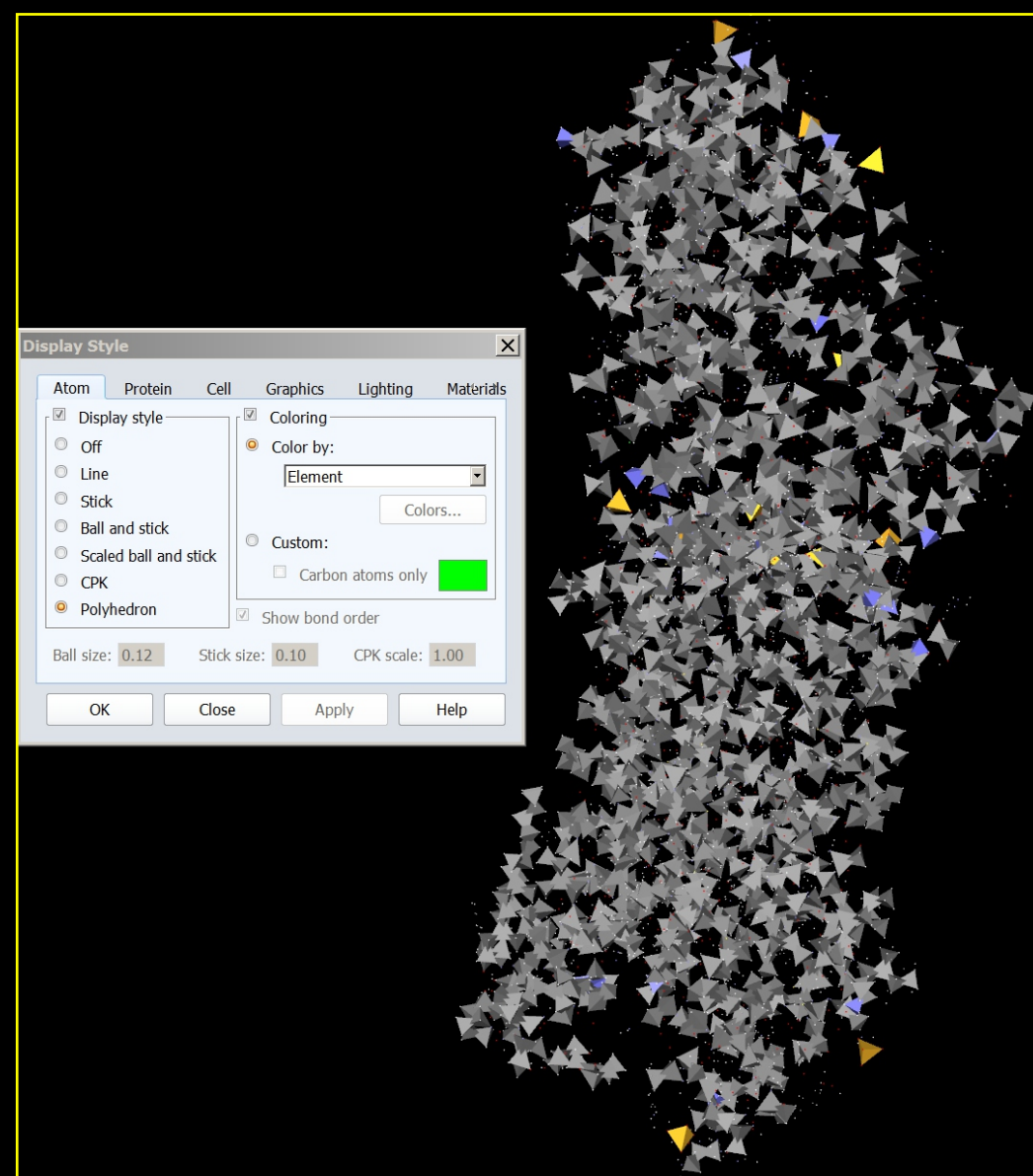
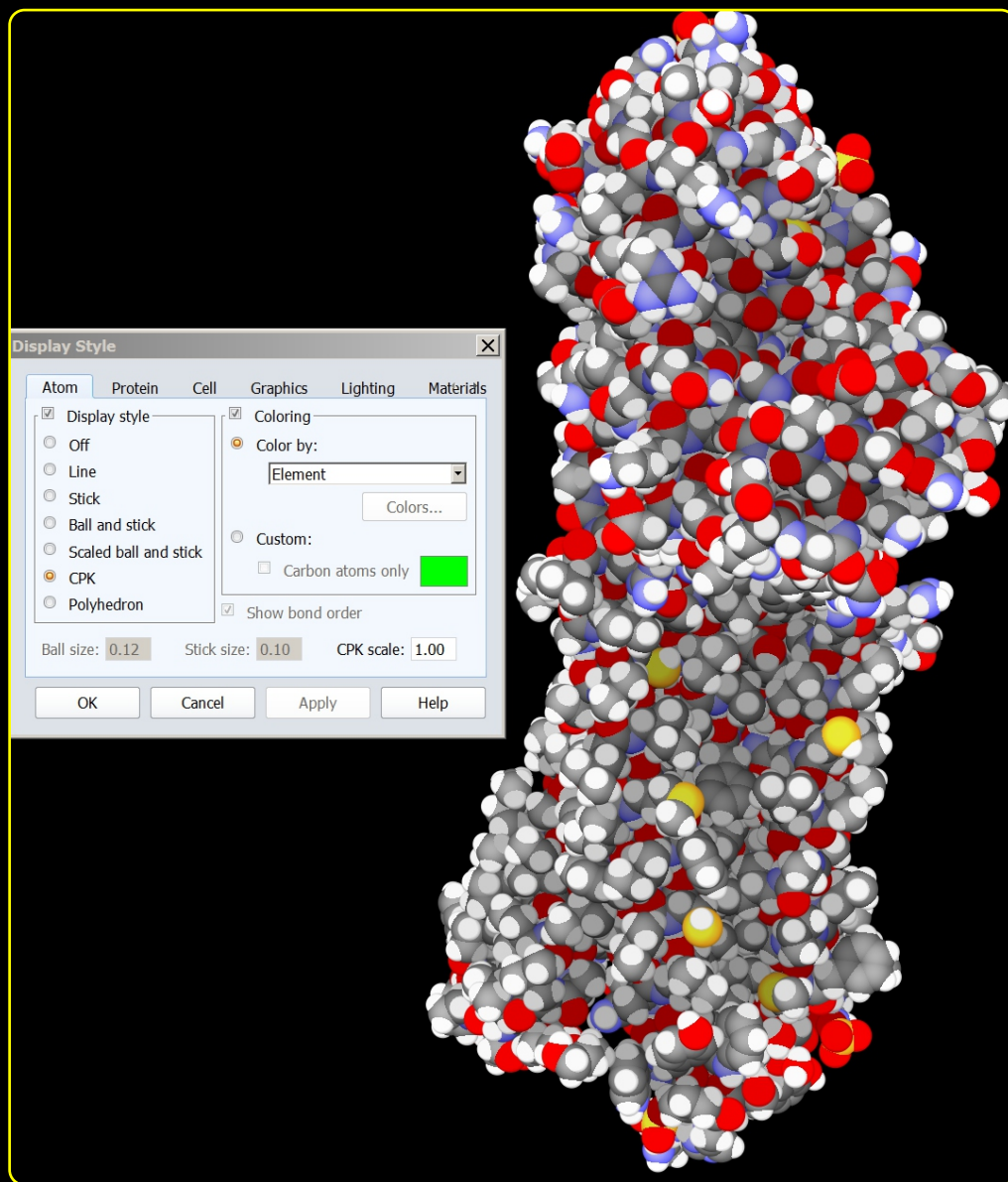
UVEĆANA SLIKA

ISPROBATI RAZLIČITE MOGUĆNOSTI PRIKAZIVANJA MOLEKULA KAO ŠTO JE PRIKAZANO NA SLEDEĆIM SLIKAMA.



UVEĆANA SLIKA

ISPROBATI RAZLIČITE MOGUĆNOSTI PRIKAZIVANJA MOLEKULA KAO ŠTO JE PRIKAZANO NA SLEDEĆIM SLIKAMA.





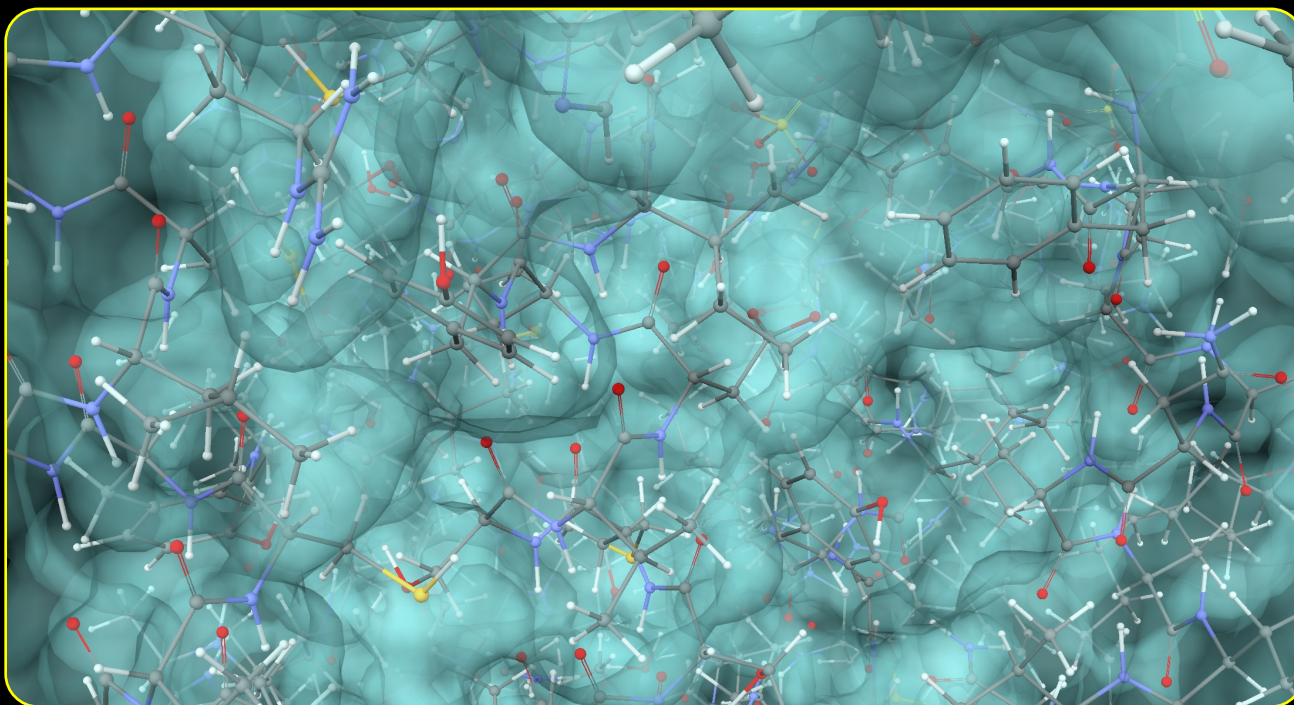
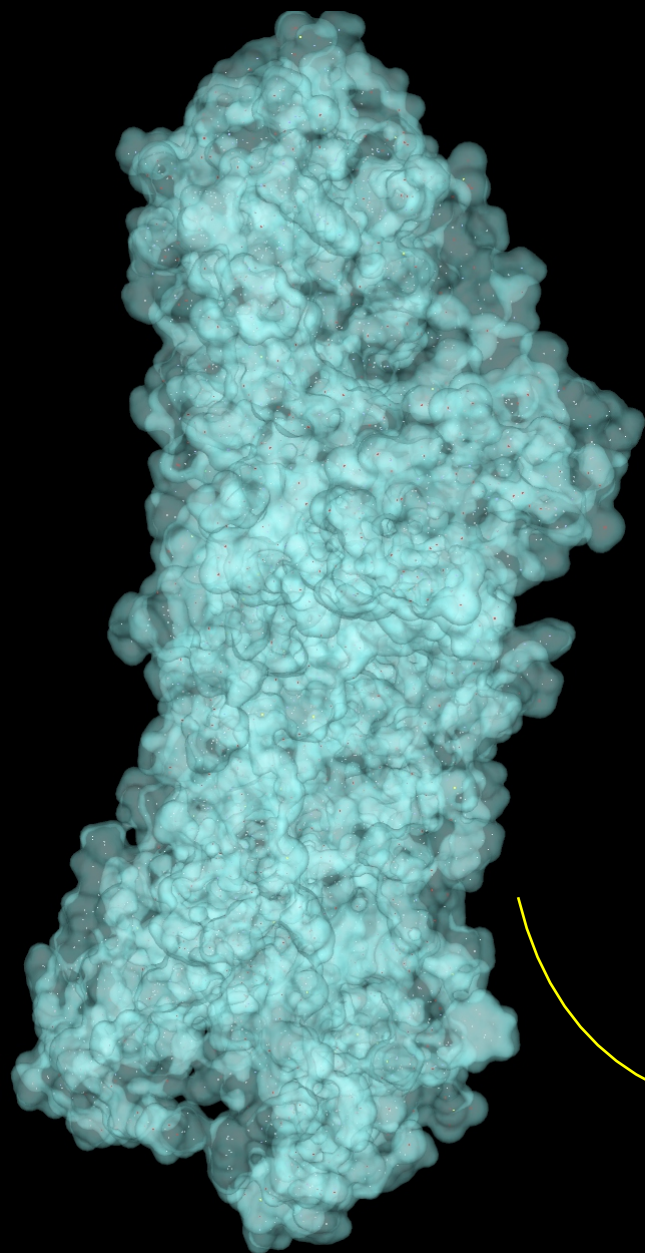
# DODAVANJE 3D POVRŠINE KOJA DEFINIŠE ZAPREMINU MOLEKULA

The image shows a screenshot of the Discovery Studio 4.1 Visualizer software interface. The main window displays a 3D molecular model of a protein-ligand complex. A context menu is open over the model, with the 'Add...' option selected, which has opened a sub-menu. In this sub-menu, the 'Add Surface' option is highlighted, and a tooltip explains: 'Add Surface: Adds a surface to the selected molecules in a Molecule Window. Click here for help'. To the right of the main window, the 'Create Surface' dialog box is open. It has several sections: 'Display style' with radio buttons for Solvent, Soft, and VDW; 'Surface rendering' with radio buttons for Solid and Wire mesh; 'Coloring' with options for 'Color by' (Atom Charge), 'By grid', and 'Custom' (with a color picker); 'Probe radius' set to 0.6; 'Transparent' and 'Opaque' sliders; 'Reverse Side' checked; and 'Type' with radio buttons for Open and Closed. The dialog also has OK, Cancel, Help, and Reset buttons.

**1. PRITISNUTI DESNO DUGME MIŠA**

**2. MOGUĆE JE RAZLIČITO PODEŠAVANJE PARAMETARA**

DODAVANJE 3D POVRŠINE KOJA DEFINIŠE ZAPREMINU MOLEKULA



UVEĆANA SLIKA

# UKLANJANJE 3D POVRŠINE

The image shows the Discovery Studio 4.1 Visualizer interface. The main window displays a 3D surface representation of a protein structure, colored in light blue. A context menu is open over the surface, listing various actions. The 'Remove Surface' option is highlighted, and a tooltip provides additional information: 'Removes surfaces from the selected molecules in a Molecule Window.' and a link to 'Click here for help'. The interface includes a menu bar (File, Edit, View, Chemistry, Structure, Sequence, Chart, Scripts, Tools, Window, Help), a toolbar with various icons, and a search bar at the top right.

Discovery Studio 4.1 Visualizer

File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help

Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools

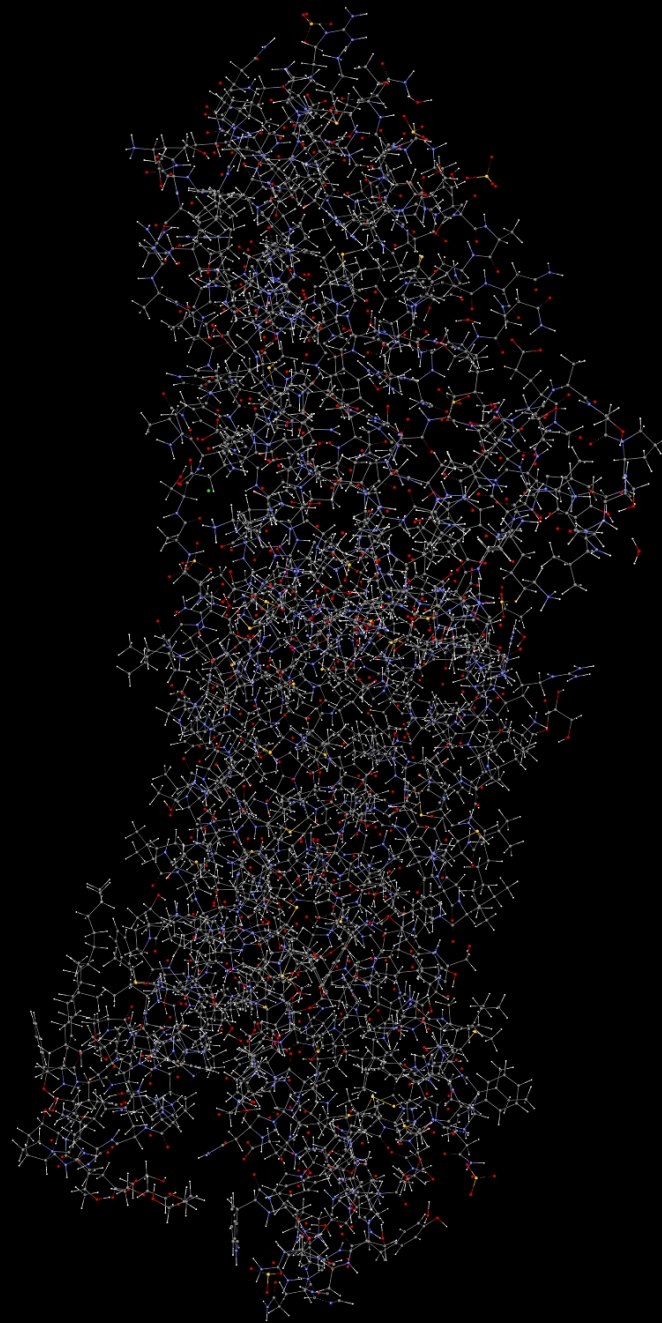
Non-bond Interactions... Search product features

4DKL

Remove Surface  
Removes surfaces from the selected molecules in a Molecule Window.  
[Click here for help](#)

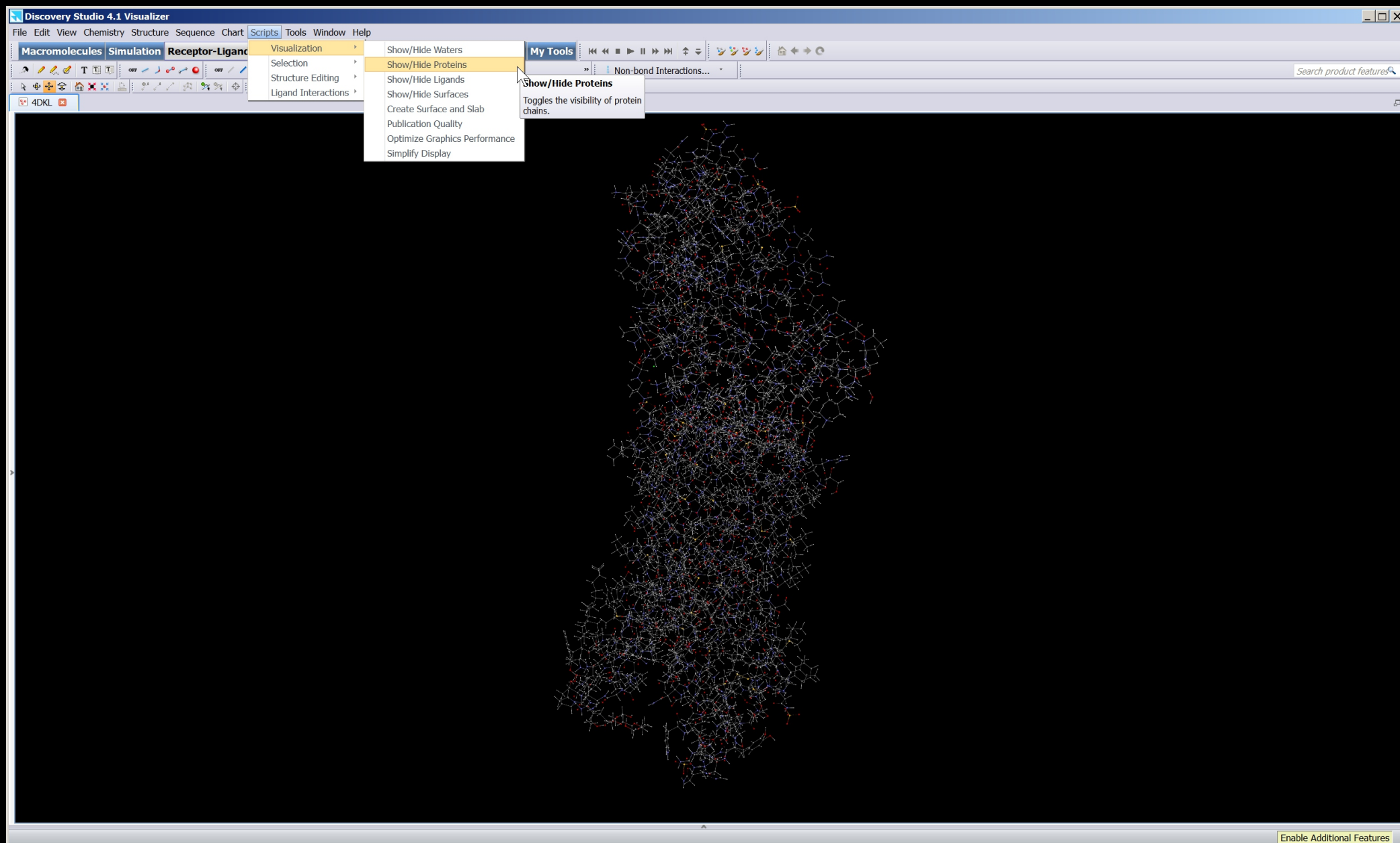
Enable Additional Features

UKLANJANJE 3D POVRŠINE - IZGLED MOLEKULA POŠTO JE 3D POVRŠINA UKLONJENA



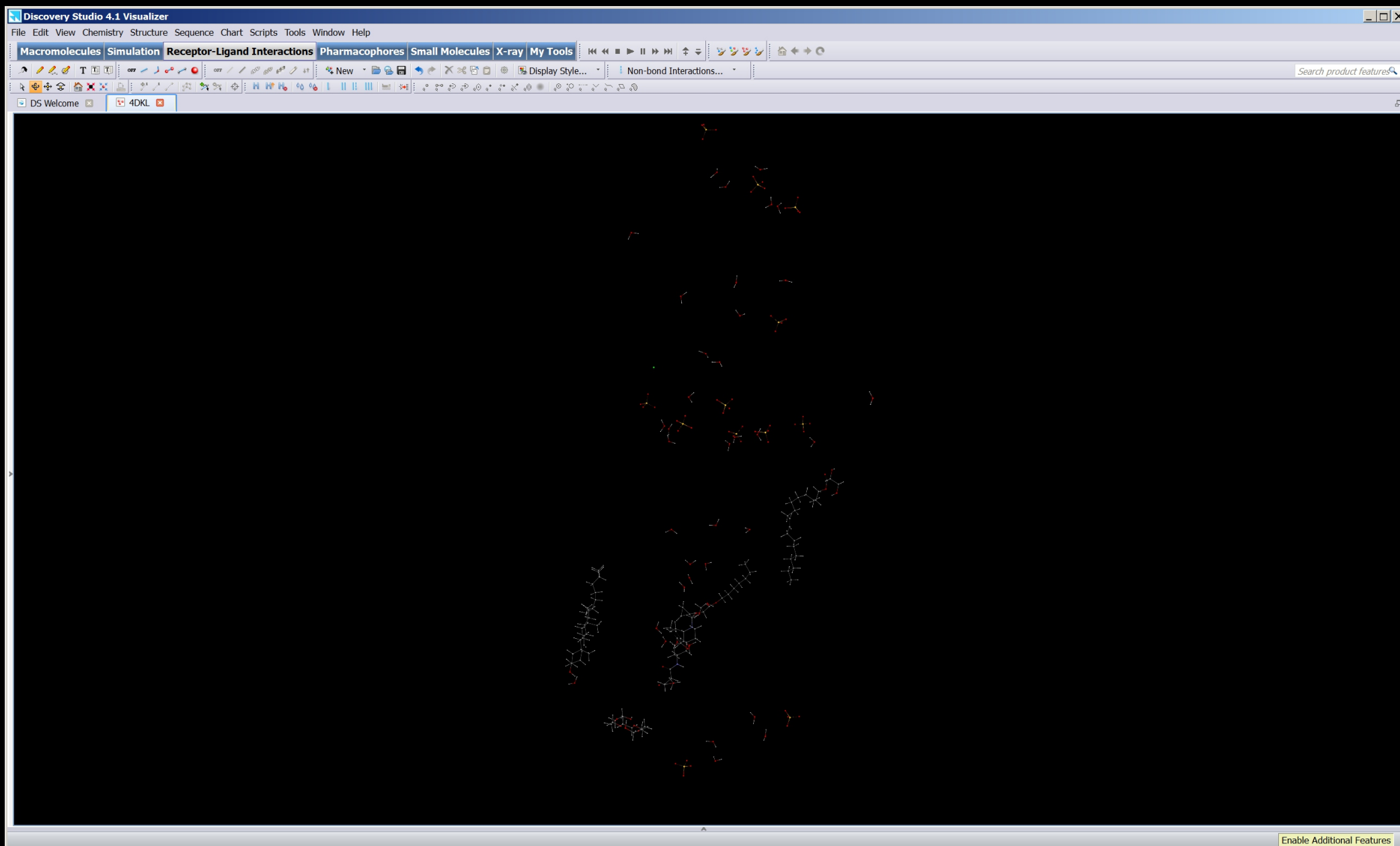
UKLANJANJE PRIKAZA ("SAKRIVANJE") POJEDINIH ELEMENATA MOLEKULA.

OPCIJA 1: PREKO MENIJA "SCRIPTS". PRIMER PRIKAZUJE UKLANJANJE PRIKAZA MOLEKULA PROTEINA.



UKLANJANJE PRIKAZA ("SAKRIVANJE") POJEDINIH ELEMENATA MOLEKULA.

OPCIJA 1: PREKO MENIJA "SCRIPTS". IZGLED EKRANA POŠTO JE "SAKRIVEN" MOLEKUL PROTEINA. (PREOSTAJU MOLEKULI VODE, JONA I LIGANADA).



UKLANJANJE I/ILI SELEKTOVANJE POJEDINIH ELEMENATA MOLEKULA.

OPCIJA 2: PREKO MENIJA "View/Hierarchy".

The image shows a screenshot of the Discovery Studio 4.1 Visualizer software interface. The main window displays a 3D molecular model of a protein-ligand complex. The protein backbone is shown in a light blue/grey color, and the ligand is shown in a stick representation with orange and red atoms. The interface includes a menu bar at the top with options: File, Edit, View, Chemistry, Structure, Sequence, Chart, Scripts, Tools, Window, Help. Below the menu bar is a toolbar with various icons for navigation and manipulation. The 'View' menu is open, showing options such as Display Style..., Color..., Transform, Spin, Storyboard, Clipping Planes..., Stereo, Tile Molecules in View (Ctrl+L), Full Screen (F11), Visibility, Graphics (Ctrl+G), Hierarchy (Ctrl+H), Data Table, Explorers, Docks, Toolbars, and Tool Panels. The 'Hierarchy' option is selected, and a tooltip is visible over it, stating: **Toggle Hierarchy View Visibility (Ctrl+H)**  
Toggles the visibility of the Hierarchy View in the current window.  
[Click here for help](#)

# SELEKTOVANJE POJEDINIH ELEMENATA MOLEKULA.

## OPCIJA 2: PREKO MENIJA "View/Hierarchy".

1. SELEKTOVATI LIGAND 1

2. SELEKTOVANI LIGAND, ŽUTO, ZUMIRANO

3. KLIKNUTI DESNIM DUGMETOM MIŠA

Discovery Studio 4.1 Visualizer

File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help

Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools

DS Welcome 4DKL

- <Cell>
- 4DKL
- A
- A
- A
- Hetatm
- Water
- Active Sites
- Protein Groups
- Ligand Groups
  - Ligand 1
  - Ligand 2
  - Ligand 3
  - Ligand 4
  - Ligand 5

Cut	Ctrl+X
Copy	Ctrl+C
Paste	Ctrl+V
Hide	
Show	
Show All	
Show Only	
Select All	Ctrl+A
Select Parents	
View	>
Mouse Mode	>
Display Style...	Ctrl+D
Color	>
Apply Forcefield	
Show Sequence	Ctrl+Q
Labels	>
Group...	

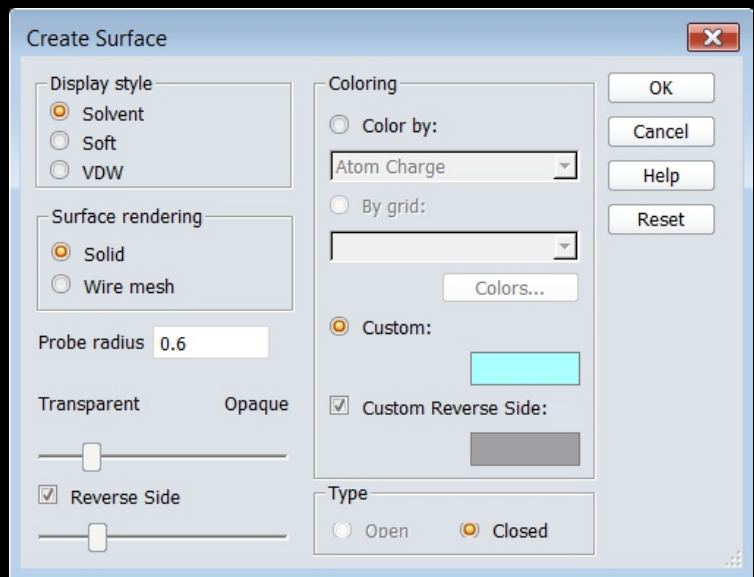
Enable Additional Features



## SELEKTOVANJE POJEDINIH ELEMENATA MOLEKULA.

OPCIJA 2: PREKO MENIJA "View/Hierarchy". PRIKAZIVANJE 3D POVRŠINE KOJA DEFINIŠE ZAPREMINU LIGANDA.

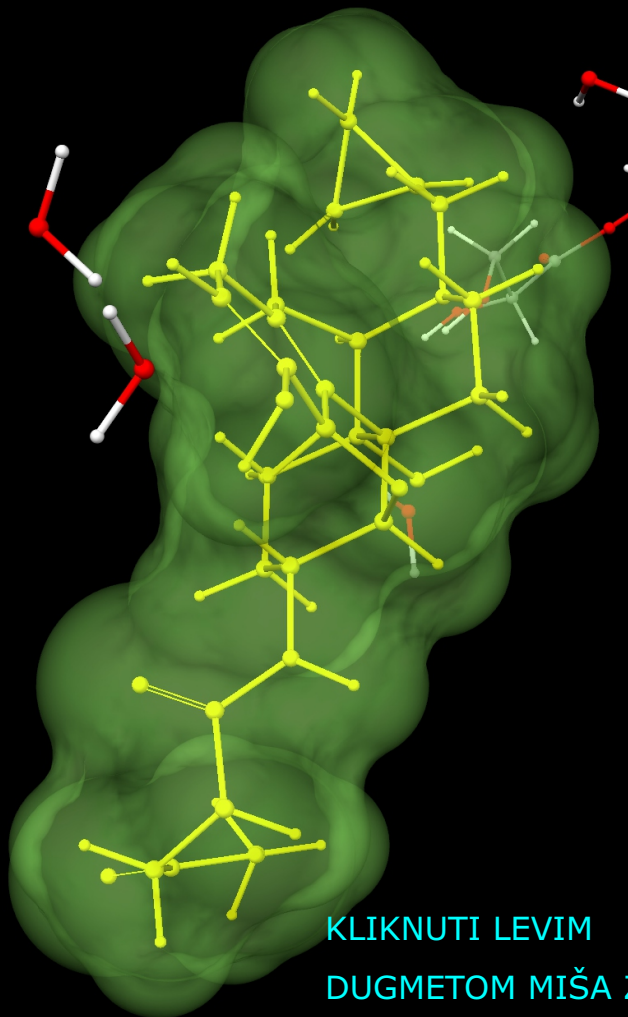
1.



**MOGUĆE JE  
RAZLIČITO  
PODEŠAVANJE  
PARAMETARA**

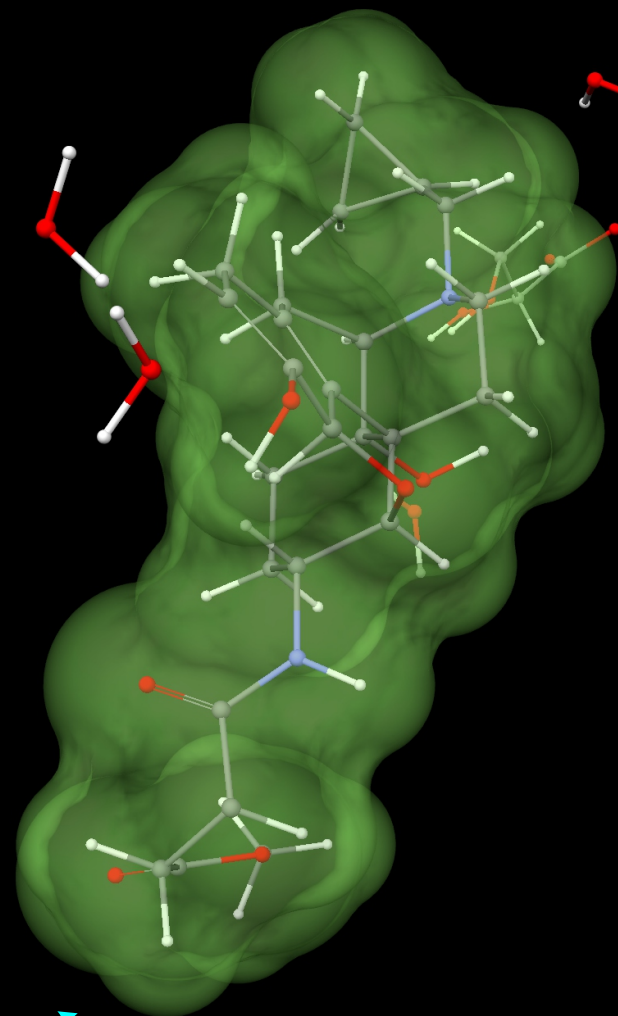
POJAVLJUJE SE  
POLUPROZIRNA,  
ZELENA SFERA KOJA  
PREDSTAVLJA  
PRIBLIŽNU ZAPREMINU  
LIGANDA

2.



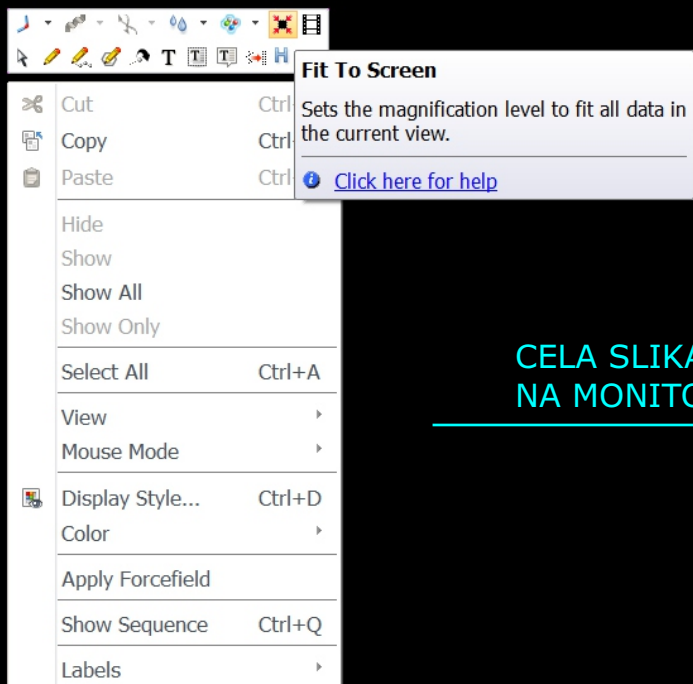
KLIKNI LEVIM  
DUGMETOM MIŠA ZA  
DESELEKTOVANJE

3.



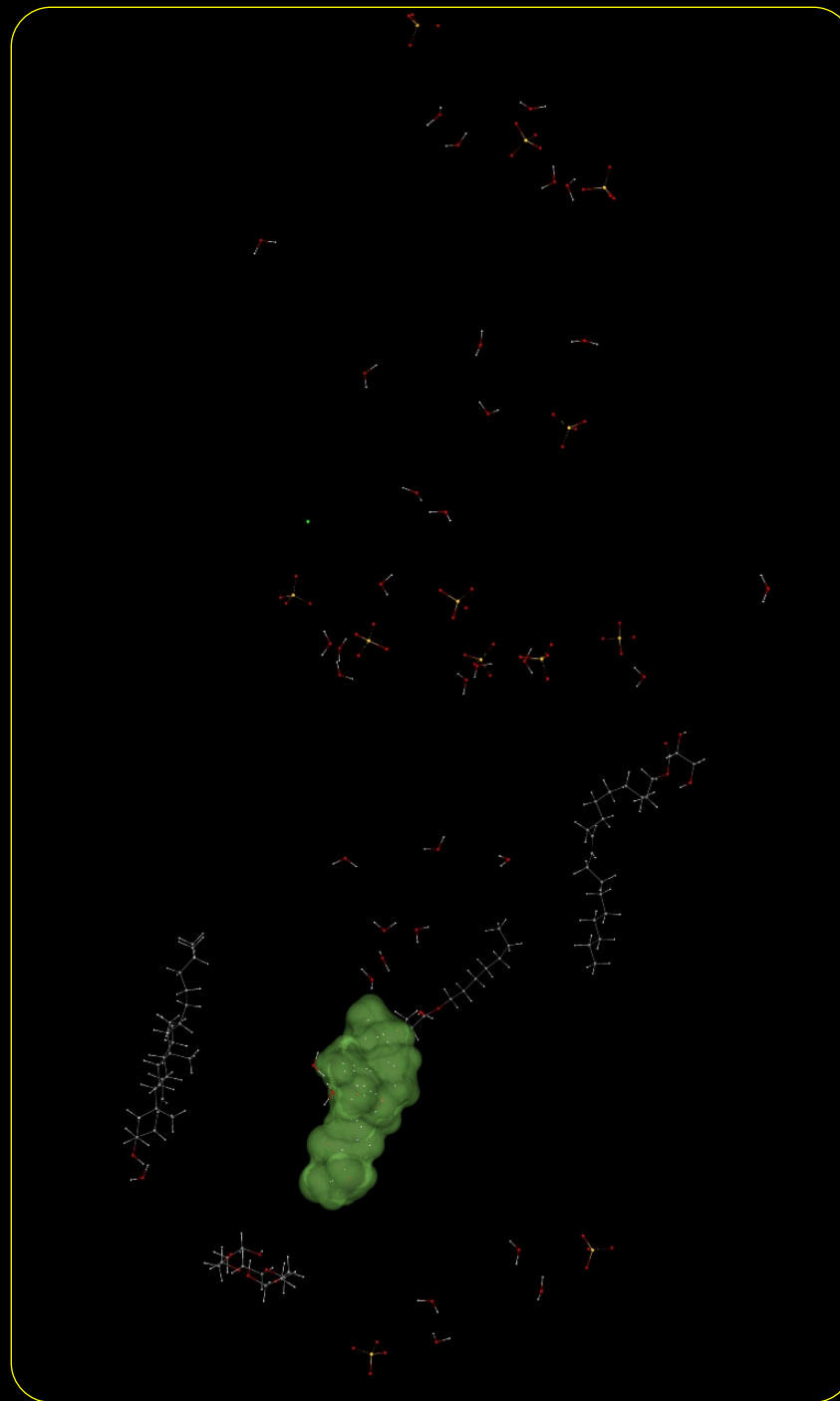
# POSTAVLJANJE CELOG MOLEKULA NA MONITOR ("U KADAR")

1.



CELA SLIKA SE VIDI  
NA MONITORU

2.



## SELEKTOVANJE POJEDINIH ELEMENATA MOLEKULA.

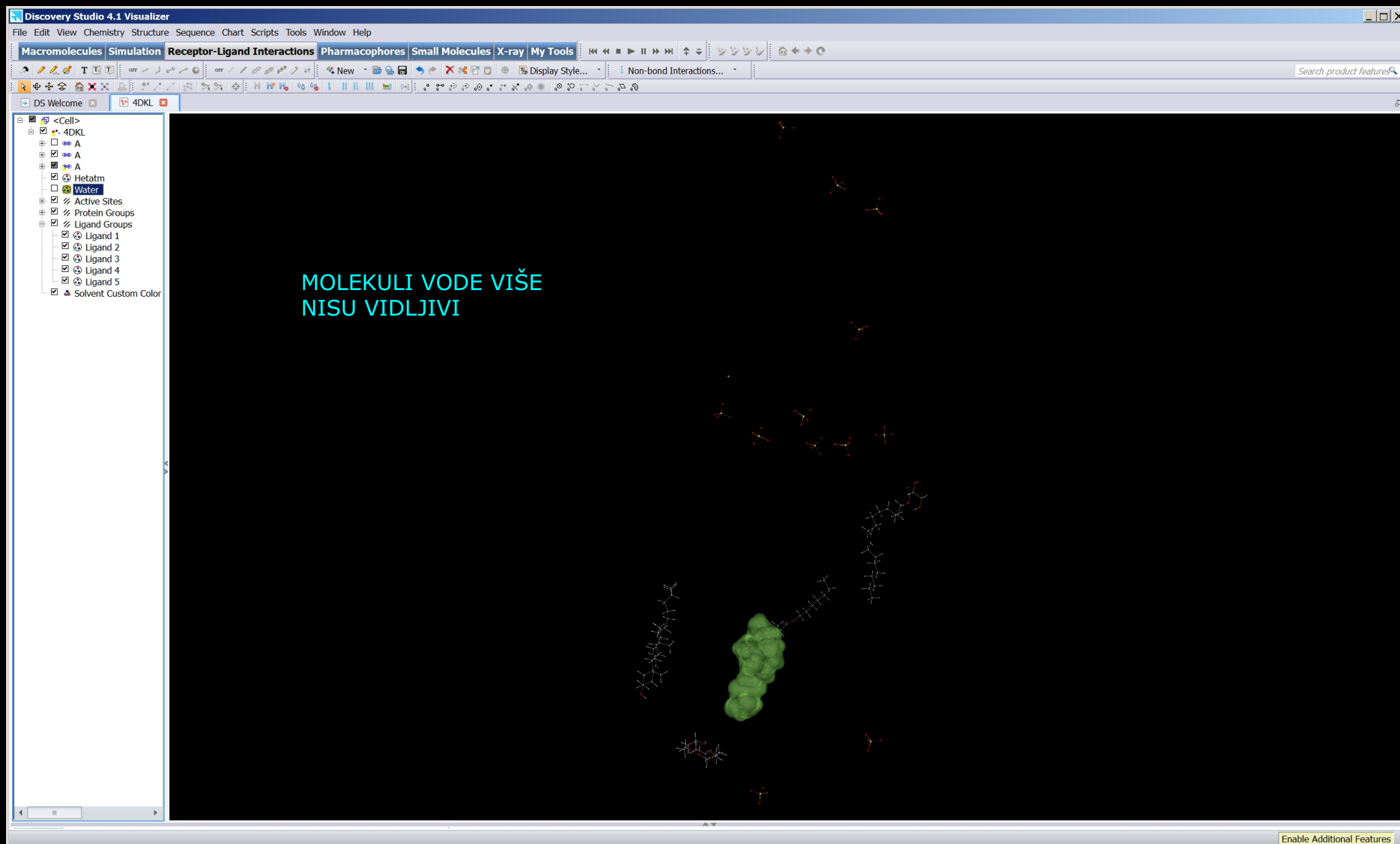
OPCIJA 2: PREKO MENIJA "View/Hierarchy". SELEKTOVANJE MOLEKULA VODE.

The screenshot displays the Discovery Studio 4.1 Visualizer interface. On the left, the Hierarchy panel is expanded to show the 'Water' molecule selected under the '4DKL' system. The main 3D view shows a protein structure with a green surface representation of a ligand and several water molecules (represented as small red and white spheres) scattered around it. A cyan arrow points from the 'Water' entry in the Hierarchy panel to the water molecules in the 3D view.

SELEKTOVATI MOLEKULE VODE, ZATIM ISKLJUČITI NJIHOV PRIKAZ NA MONITORU

## SELEKTOVANJE POJEDINIH ELEMENATA MOLEKULA.

OPCIJA 2: PREKO MENIJA "View/Hierarchy". UKLANJANJE PRIKAZA ("SAKRIVANJE") MOLEKULA VODE.



## SELEKTOVANJE POJEDINIH ELEMENATA MOLEKULA.

OPCIJA 2: PREKO MENIJA "View/Hierarchy". MOLEKULI VODE SU "SAKRIVENI" DOK JE MOLEKUL PROTEINA PONOVO VIDLJIV JER SU SELEKTOVANE OPCIJE ZAKRUŽENE LJUBIČATIM PRAVOUGAONICIMA. SLEDI SUKCESIVNO SELEKTOVANJE LIGANADA 2-5 I PRIKAZIVANJE NJIHOVIH 3D POVRŠINA.

**1.** SELEKTOVATI LIGAND 2, ZATIM PONOVI TI SVE OPERACIJE KAO ZA LIGAND 1

**2.**

Discovery Studio 4.1 Visualizer

File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help

Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools

DS Welcome 4DKL\_1

<Cell>  
4DKL  
A  
A  
A  
Hetatm  
Water  
Active Sites  
Protein Groups  
Ligand Groups  
Ligand  
Ligand  
Ligand  
Ligand  
Solvent

Cut Ctrl+X  
Copy Ctrl+C  
Paste Ctrl+V  
Hide  
Show  
Show All  
Show Only  
Select All Ctrl+A  
Select Parents  
Invert Selection  
View  
Display Bonds  
Group...  
Remove Group

Create Surface

Display style  
 Solvent  
 Soft  
 VDW

Surface rendering  
 Solid  
 Wire mesh

Probe radius 0.6

Transparent Opaque

Reverse Side

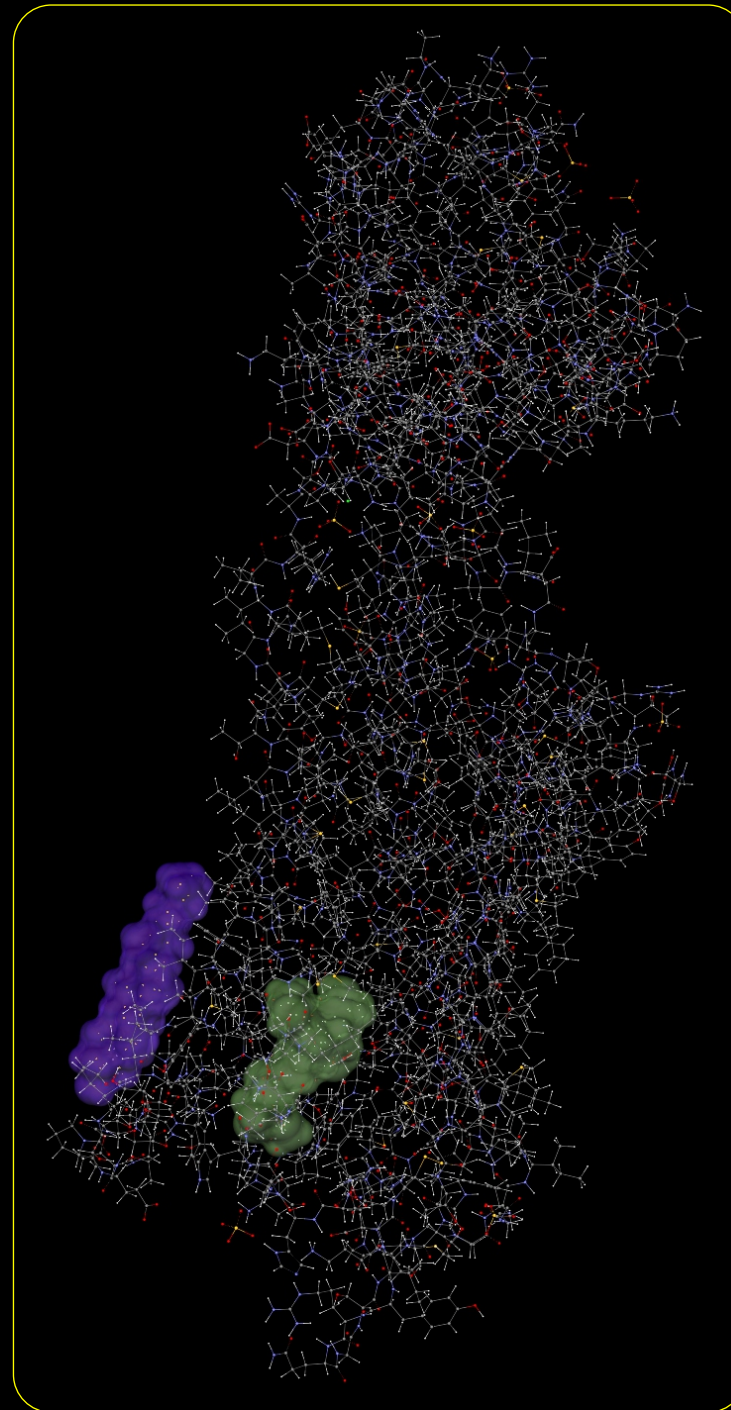
Coloring  
 Color by:  
Atom Charge  
 By grid:  
Colors...  
 Custom:  
Custom Reverse Side:  
Type  
 Open  Closed

OK  
Cancel  
Help  
Reset

29/35 Enable Additional Features

SELEKTOVANJE POJEDINIH  
ELEMENTA MOLEKULA.

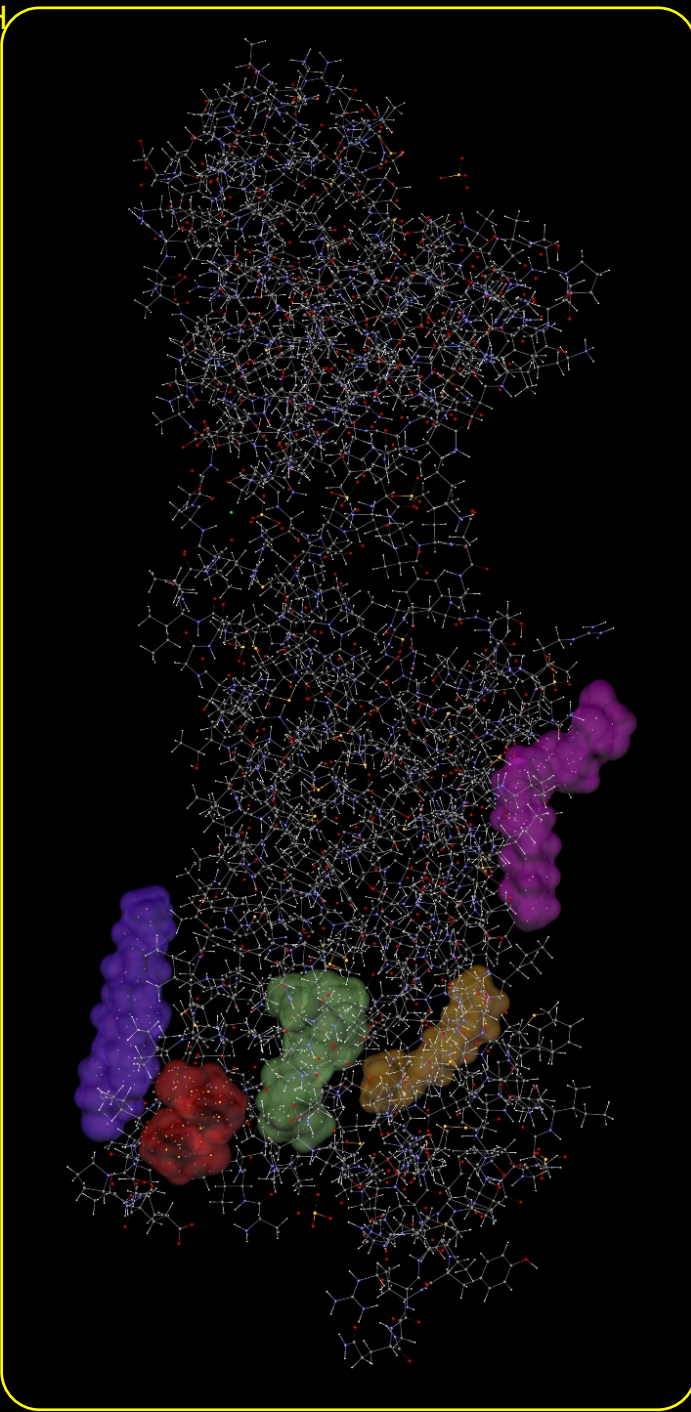
IZGLED  
MAKROMOLEKULA  
(PROTEINA) SA  
2 LIGANADA,  
PRIKAZANA SA  
POLUPROZIRNIM  
ZAPREMINAMA. BOJE SU  
PROIZVOLJNE.



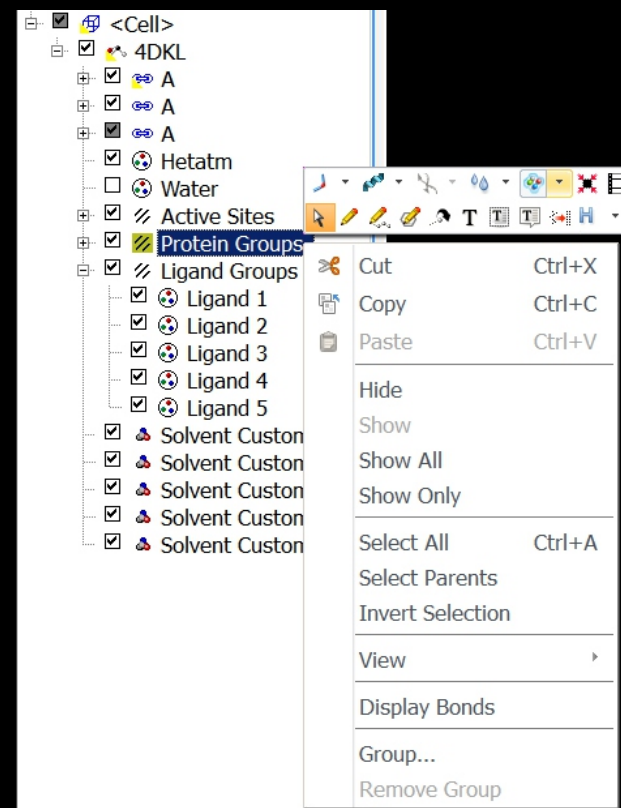
PONOVITI ISTE OPERACIJE  
ZA LIGANDE 3,4 I 5, KORISTEĆI  
RAZLIČITE BOJE

SELEKTOVANJE POJEDINI  
ELEMENTA MOLEKULA.

IZGLED  
MAKROMOLEKULA  
(PROTEINA) SA SVIH  
5 LIGANADA,  
PRIKAZANIH SA  
POLUPROZIRNIM  
ZAPREMINAMA. BOJE SU  
PROIZVOLJNE.



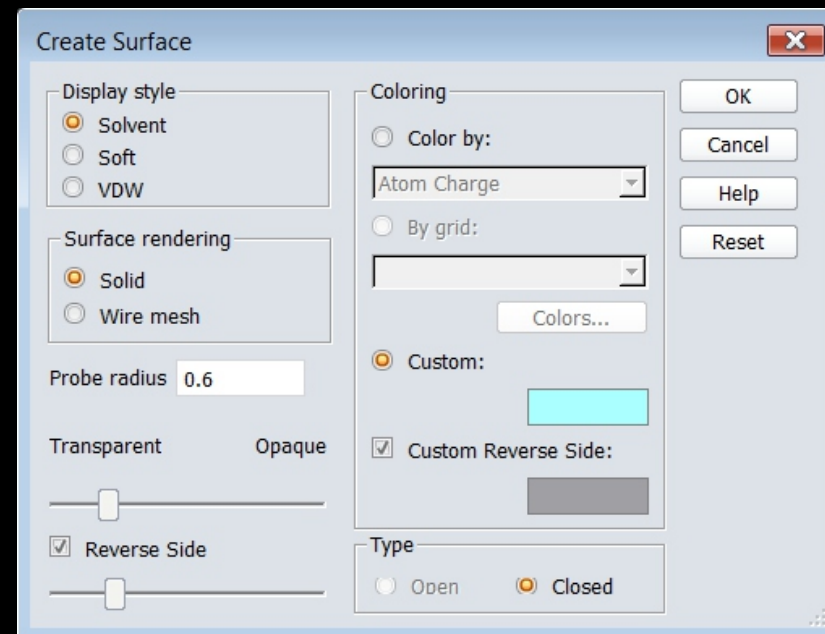
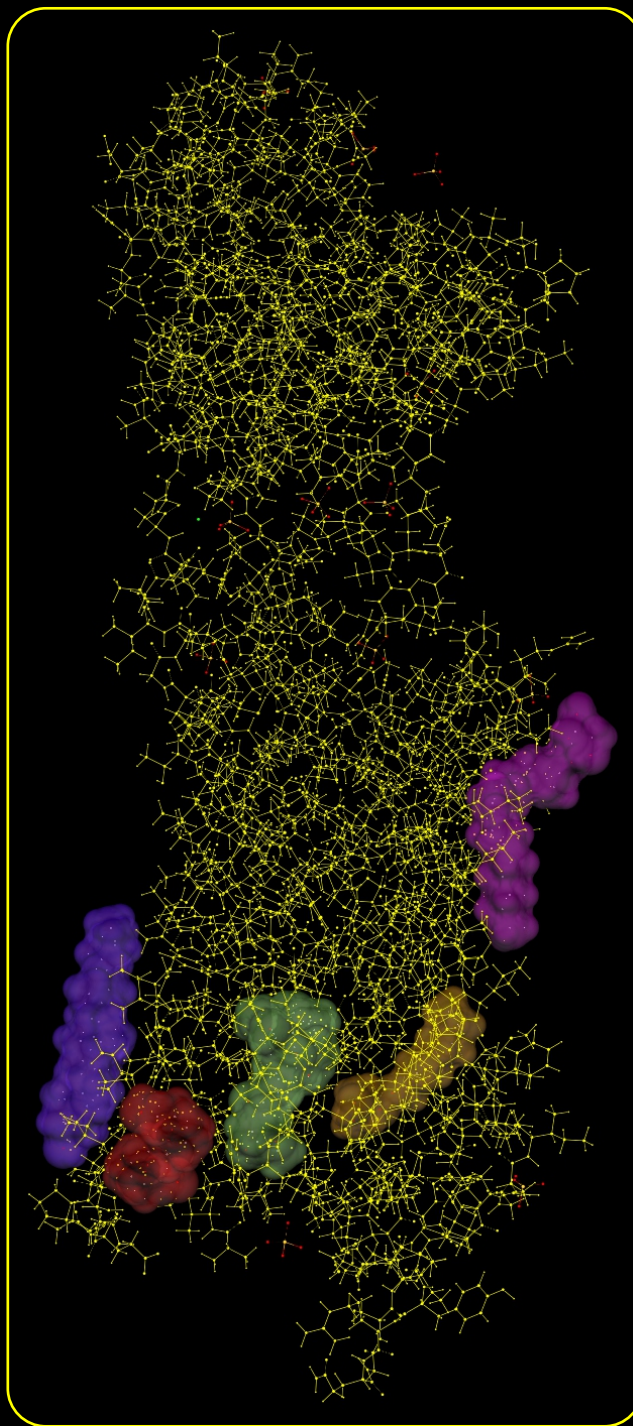
ZATIM  
SELEKTOVATI  
MOLEKUL  
PROTEINA



A screenshot of a software interface showing a hierarchical tree of molecular components. The tree is titled '<Cell>' and contains the following items: 4DKL, A, A, A, Hetatm, Water, Active Sites, Protein Groups (highlighted), Ligand Groups, Ligand 1, Ligand 2, Ligand 3, Ligand 4, Ligand 5, Solvent Custom, Solvent Custom, Solvent Custom, Solvent Custom, and Solvent Custom. A context menu is open over the 'Protein Groups' item, showing options: Cut (Ctrl+X), Copy (Ctrl+C), Paste (Ctrl+V), Hide, Show, Show All, Show Only, Select All (Ctrl+A), Select Parents, Invert Selection, View, Display Bonds, Group..., and Remove Group.

SELEKTOVANJE POJEDINI  
ELEMENATA MOLEKULA.

IZGLED  
SELEKTOVANOG  
MOLEKULA  
PROTEINA

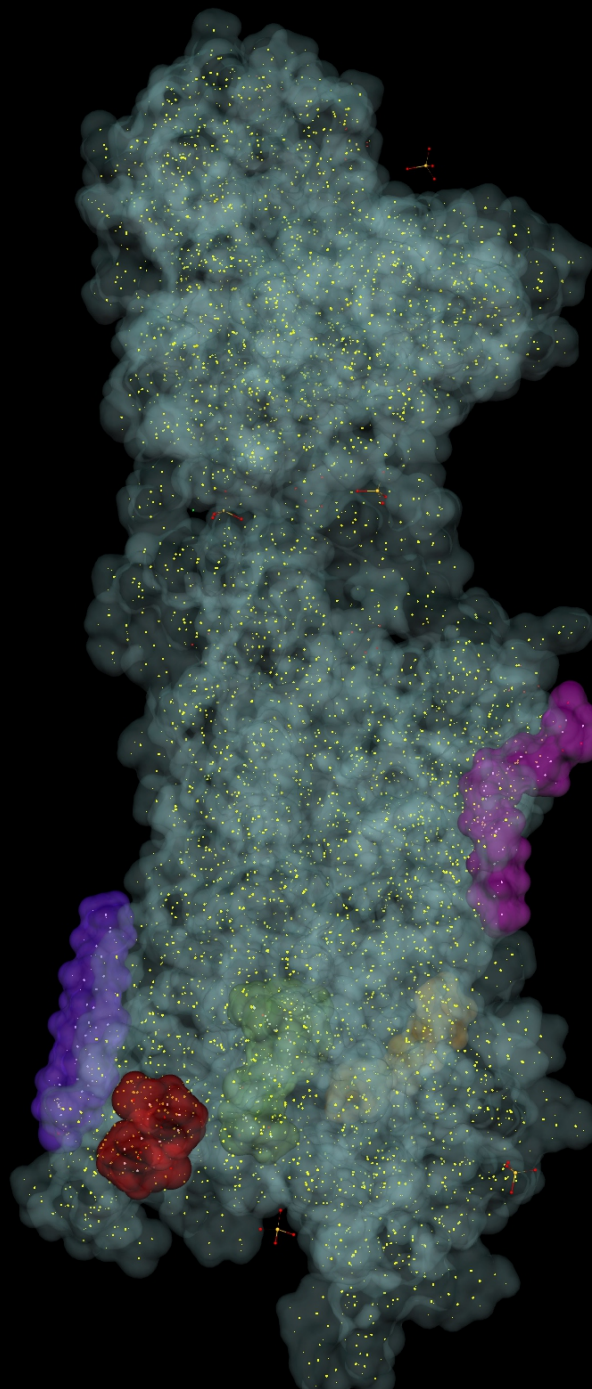


PRIKAZATI 3D POVRŠINU (ZAPREMINU)  
MOLEKULA PROTEINA



SELEKTOVANJE POJEDINI  
ELEMENTA MOLEKULA.

IZGLED SELEKTOVANOG  
MOLEKULA PROTEINA  
SA 3D POVŠINOM KAO I  
3D POVRŠINAMA SVAKOG  
LIGANDA. MOLEKULI VODE NISU  
VIDLJIVI, ALI SE VIDE JONI  
( $\text{SO}_4^{2-}$ ).

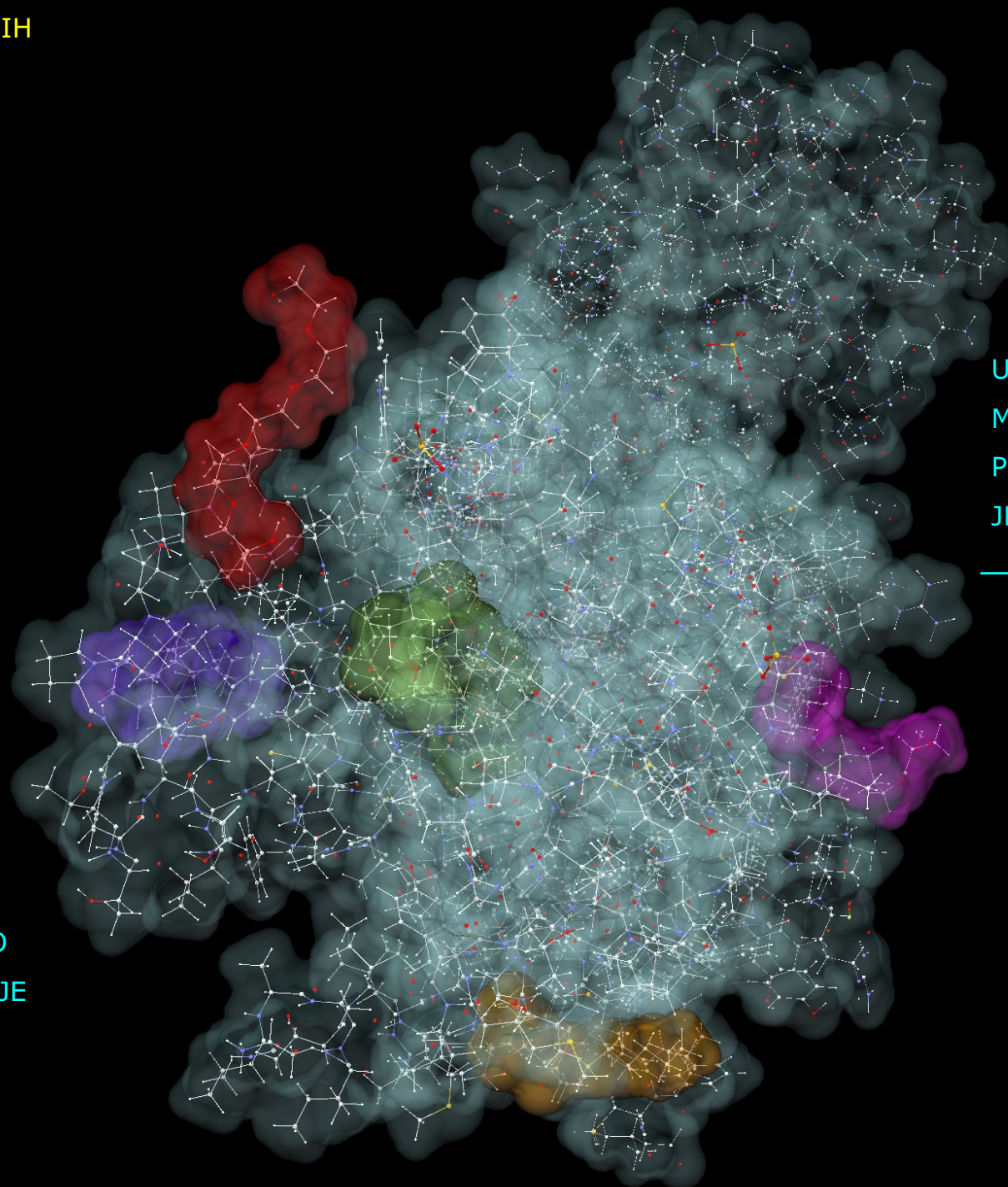


POSLE DESELEKTOVANJA,  
MOLEKUL KAO CELINA SE  
MOŽE SLOBODNO ROTIRATI,  
KORIŠĆENJEM IKONE:



MOGUĆE SU I DRUGE OPCIJE, KAO  
POMERANJE, ZUMIRANJE I DR.

SELEKTOVANJE POJEDINI  
ELEMENTA MOLEKULA.

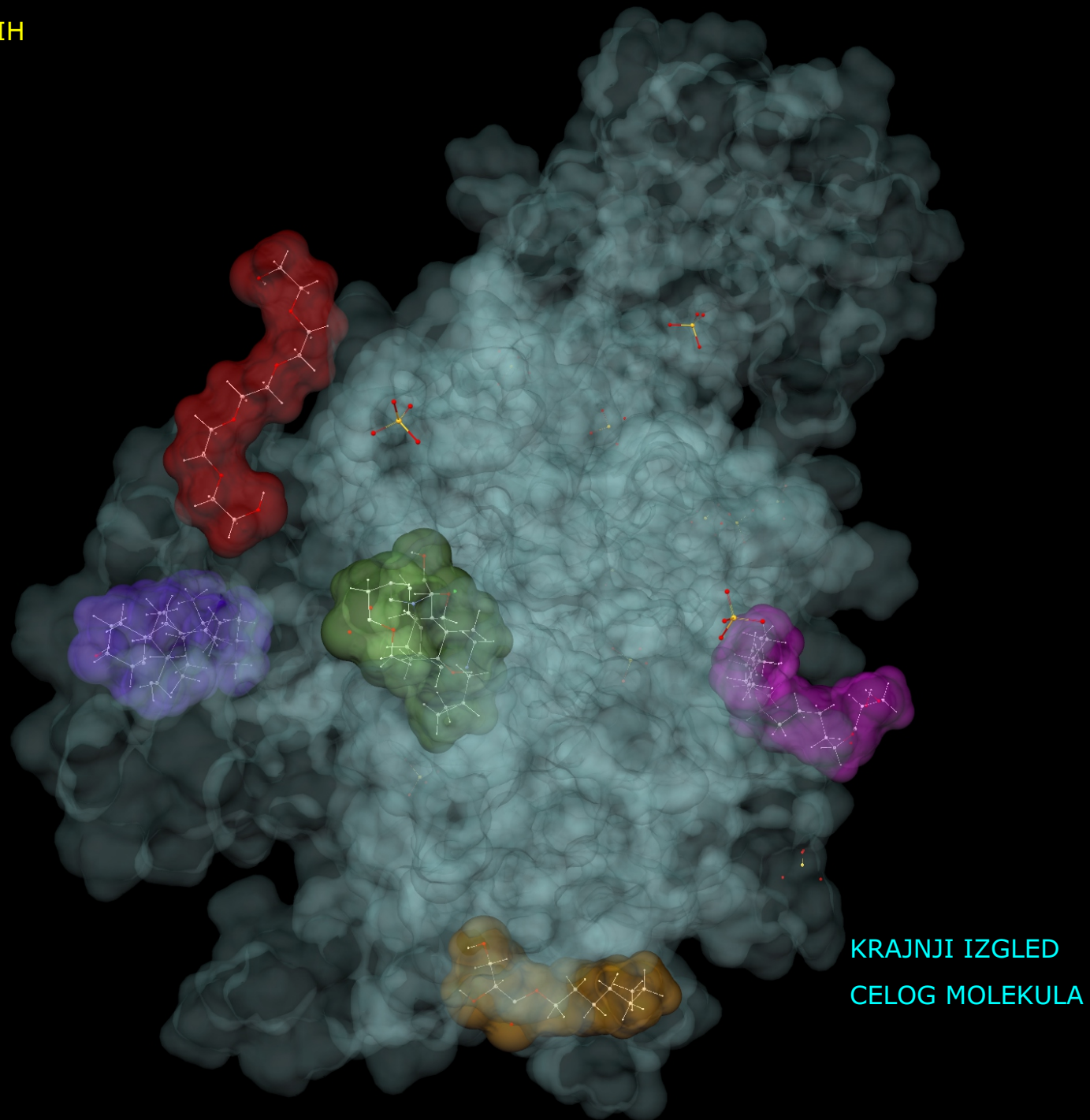


UKLONITI PRIKAZ  
MOLEKULA  
PROTEINA, KAO ŠTO  
JE RANIJE OBJAŠNJENO



IZGLED MOLEKULA KAO  
CELINE POSLE ROTACIJE

SELEKTOVANJE POJEDINI  
ELEMENATA MOLEKULA.



KRAJNI IZGLED  
CELOG MOLEKULA