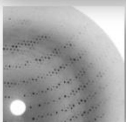
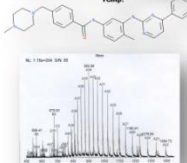
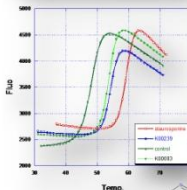
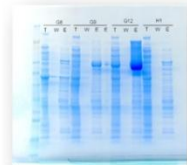


Slides and ActiveICM

Gather Data

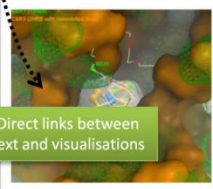
```
carboxyl_reductase_3 [Homo sapiens]  
->GLI KIQDQGLI KVF (HE_001227.1) carboxyl_  
reductase_3 [Homo sapiens]  
MSKICDVALYNNRNTDLSLAEELGQDFQDFVLTNR  
EVAHQGAAVQGLQAGSLPFRHQLDELDLQEI  
RALKLFLAKETVGLAYLVDAVAVKEDEPFPIIKAE  
RFLAKETVATVQKICELLPALDQKNSGVYVTCGL
```



Interpret, Integrate and Annotate

Structural Basis For Substrate Specificity in
Human Membrane Carboxyl Reductase
by Li Sheng¹, Frank H. Heese¹, Chen-Hua Lee¹, Hsuan-
Chang¹, James R. Swales¹, George Knebel¹, Hsuan-
Lai¹, Hsin-Yang Hsieh¹, Edward Hsueh¹, and Jan
M. Chalovich^{1,2*}

Text annotation
+
Direct links between
text and visualisations

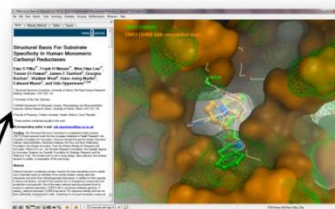


3D visualisations,
annotations
and animations

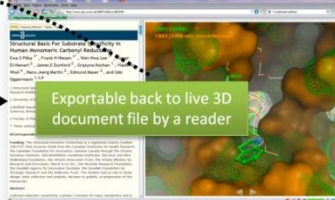


One File:
3D document:
live data of
various types

Publish and Share

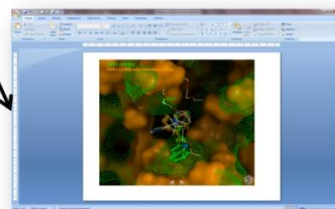


Standalone - ICM Browser
Live molecules, spreadsheets and plots,
chemistry, sequence alignments e.t.c.



Exportable back to live 3D
document file by a reader

Web – activeICM

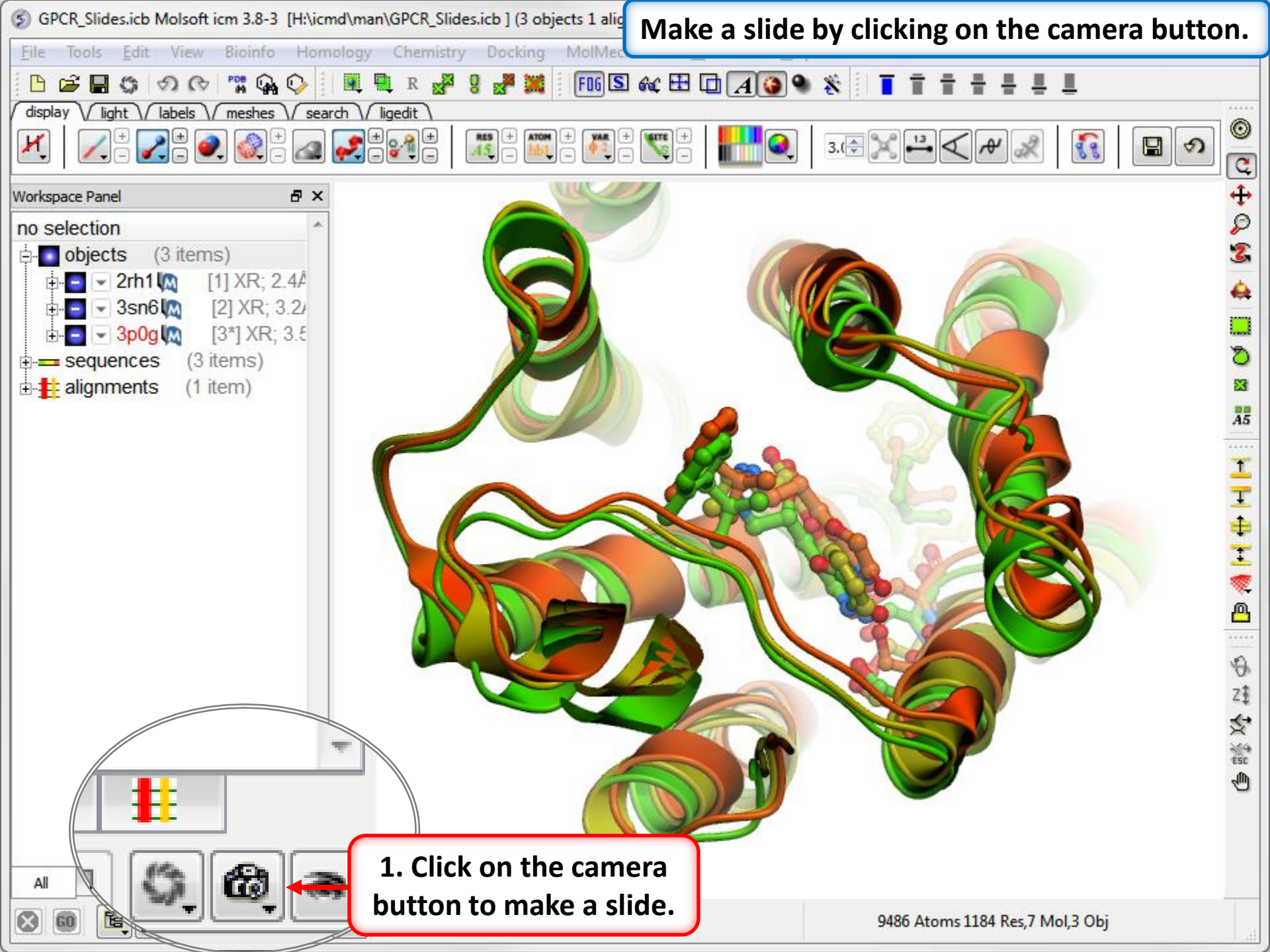


Office – activeICM
Microsoft PowerPoint, Word



In this example we are going to look at the effect of an agonist binding to the Beta-2-Adrenergic GPCR (B2AR). A prepared ICM file containing three B2AR GPCRs superimposed can be downloaded here ftp.molsoft.com/pub/GPCR_slides.icb. The file contains pdb files 2RH1 (R inactive state), 3POG (R* active state, with G-alpha mimic), and 3SN6 (R*G G-protein signalling state). The agonist ligand causes Helix 5 to shift inwards and Helix 6 to swing outwards. This agonist binding poses were predicted using ICM a year before the crystal structures were solved (see Katritch and Abagyan TIPS 2011).

Make a slide by clicking on the camera button.



1. Click on the camera button to make a slide.

The slide will be stored in the ICM workspace.

GPCR_Slides.icb Molsoft icm 3.8-3 [H:\icmd\man\GPCR_Slides.icb *] (3 objects 1 a

File Tools Edit View Bioinfo Homology Chemistry Docking MolM

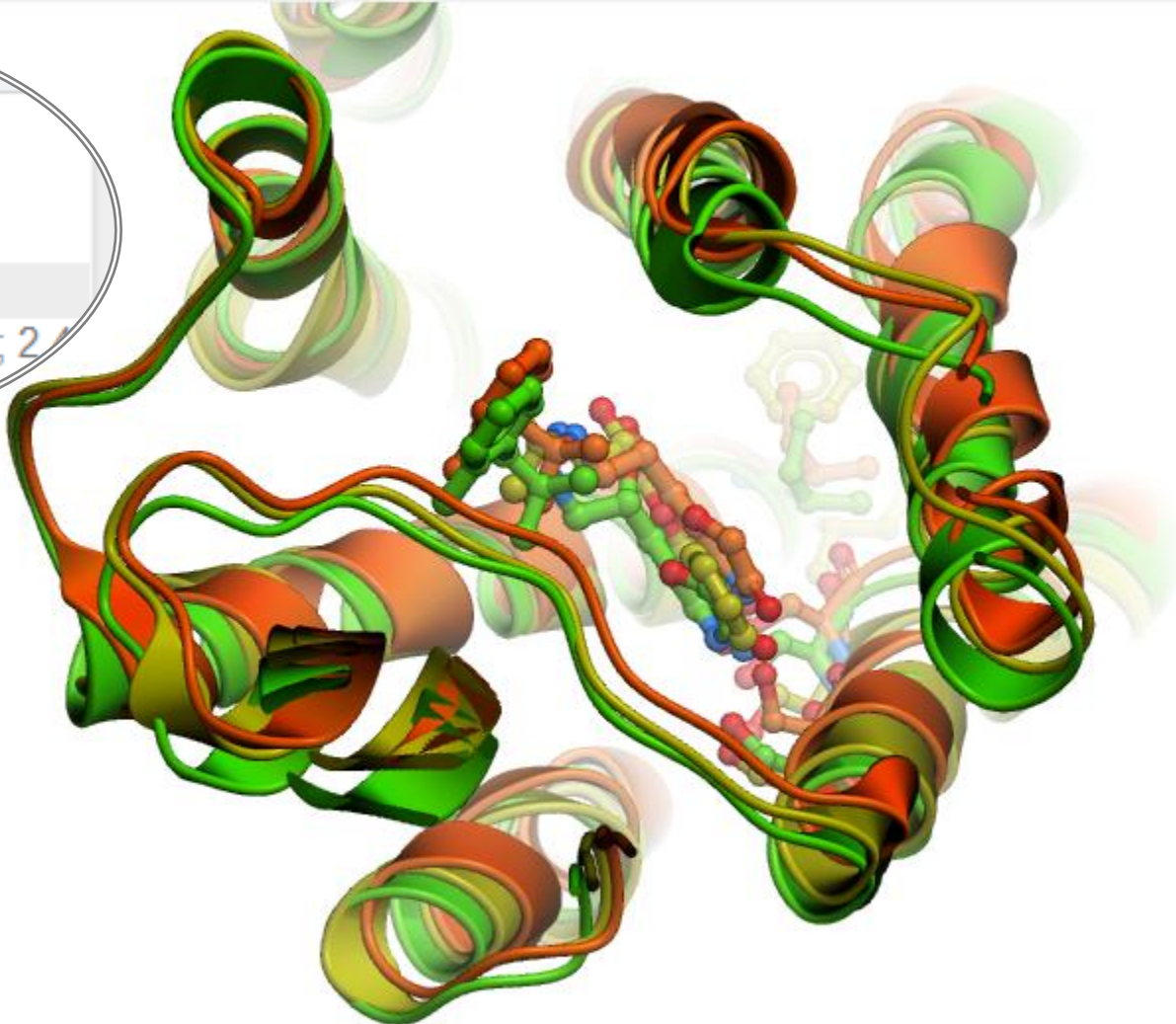
display light labels meshes search ligedit

RES 45 ATOM 111 VAR 0 SITE 0

Workspace Panel

no selection

- slides (1 item)
 - slideshow
 - 1 Slide 1
- objects (3 items)
 - 2rh1 [1] XR; 2
 - 3sn6 [2] YF
- alignments



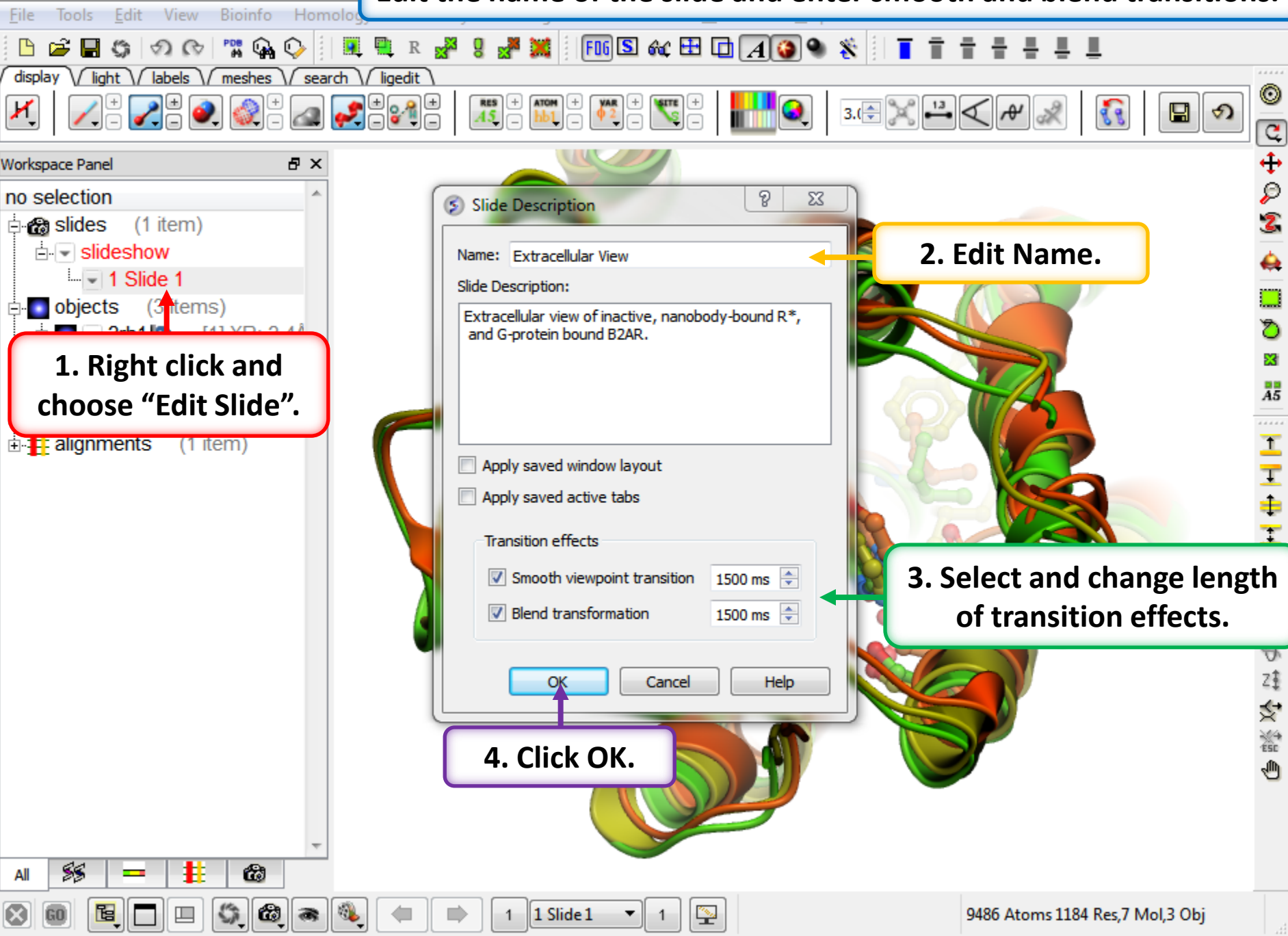
All

GO

1 1 Slide 1 1

9486 Atoms 1184 Res,7 Mol,3 Obj

Edit the name of the slide and enter smooth and blend transitions.



You can also save viewpoints to help make other slides in the same orientation.

The screenshot displays a molecular visualization software interface. The main window shows a protein structure rendered as a ribbon, with different parts colored in green, orange, and red. The structure is semi-transparent, revealing internal components. The interface includes a top menu bar with 'File', 'Tools', and 'Edit'. Below the menu is a toolbar with various icons for file operations, display settings, and navigation. A 'Workspace Panel' is visible on the left side, containing a tree view of the current scene. The tree view shows a hierarchy: 'no selection' at the top, followed by 'viewpoints (1 item)' which contains 'Extracellular_ViewPoint'. Below this are 'slides (1 item)' containing a 'slideshow' with '1 Extracellular View'. The 'objects' section lists three items: '2rh1 [1] XR; 2.4Å', '3sn6 [2] XR; 3.2Å', and '3p0g [3*] XR; 3.5Å'. There are also 'sequences (3 items)' and 'alignments (1 item)'. A red callout box points to an eye icon in the bottom toolbar, labeled '1. Click here to save a viewpoint.'. A yellow callout box points to the 'Extracellular_ViewPoint' entry in the workspace panel, labeled '2. Viewpoints are stored here.'. The bottom status bar shows '9486 Atoms 1184 Res,7 Mol,3 Obj'.

2. Viewpoints are stored here.

1. Click here to save a viewpoint.

9486 Atoms 1184 Res,7 Mol,3 Obj

Make another slide of the inward shift of Helix 5 when an agonist binds.

The image shows a screenshot of a molecular visualization software interface. The main window displays a 3D ribbon representation of a protein structure. A specific helix, labeled "H5", is highlighted in orange. A red callout box with a white background and a red border contains the text "1. Click on the camera button to make a slide." with a red arrow pointing to a camera icon in the bottom toolbar. The interface includes a top menu bar with "File", "Tools", "Edit", "View", and "Bioinfo". Below the menu is a toolbar with various icons for file operations, display settings, and search. A "Workspace Panel" on the left side shows a tree view with "no selection", "viewpoints (1 item)", "slides (1 item)", "objects (3 items)", "sequences (3 items)", and "alignments (1 item)". The "slides" folder is expanded, showing "1 Extracellular View" and "2 H5 Inward Shift". The "objects" folder contains three items: "2rh1 [1] XR; 2.4Å", "3sn6 [2] XR; 3.2Å", and "3p0g [3*] XR; 3.5Å". The bottom status bar displays "9486 Atoms 1184 Res,7 Mol,3 Obj".

1. Click on the camera button to make a slide.

Make a slide of the side chain changes of I121 and F282.

The screenshot displays the PyMOL molecular visualization software interface. The main window shows a protein structure with side chains I121 and F282 highlighted in orange and green. The workspace panel on the left lists various objects and slides. The status bar at the bottom indicates 9486 Atoms, 1184 Res, 7 Mol, 3 Obj.

Workspace Panel:

- no selection
- viewpoints (1 item)
 - Extracellular_ViewPoint
- slides (1 item)
 - slideshow
 - 1 Extracellular View
 - 2 H5 Inward Shift
 - 3 Ile121 and Phe282
- objects (3 items)
 - 2rh1 [1] XR; 2.4Å
 - 3sn6 [2] XR; 3.2Å
 - 3p0g [3*] XR; 3.5Å
- sequences (3 items)
- alignments (1 item)

Bottom Toolbar:

- All
- GO
- Camera button (indicated by a red arrow)
- Other navigation and utility icons

Status Bar: 9486 Atoms 1184 Res,7 Mol,3 Obj

1. Click on the camera button to make a slide.

Make a slide of the helix 6 swing.

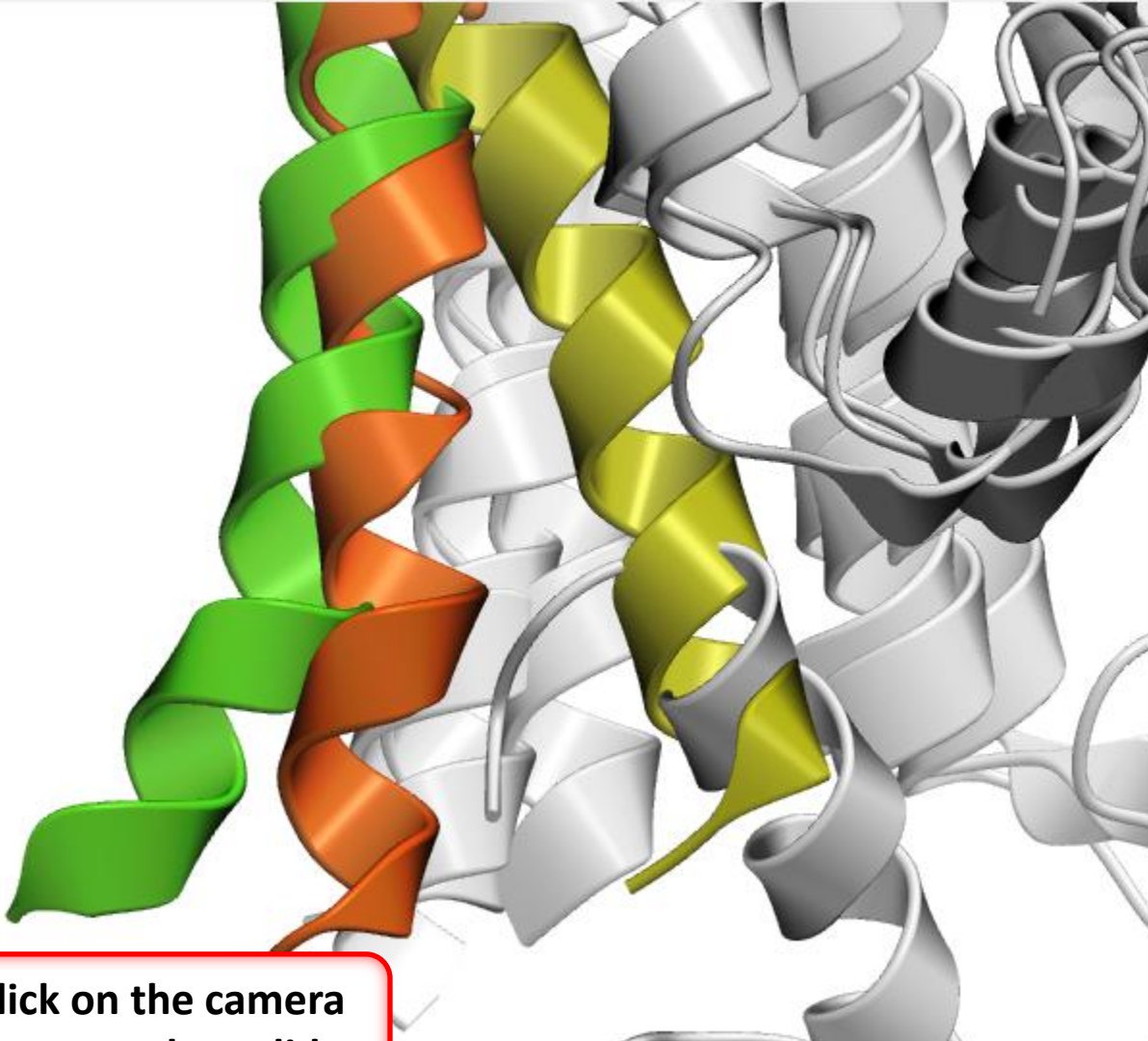
File Tools Edit View Bioinfo Homology Chemistry Docking MolMechanics Windows

display light labels meshes search ligedit

Workspace Panel

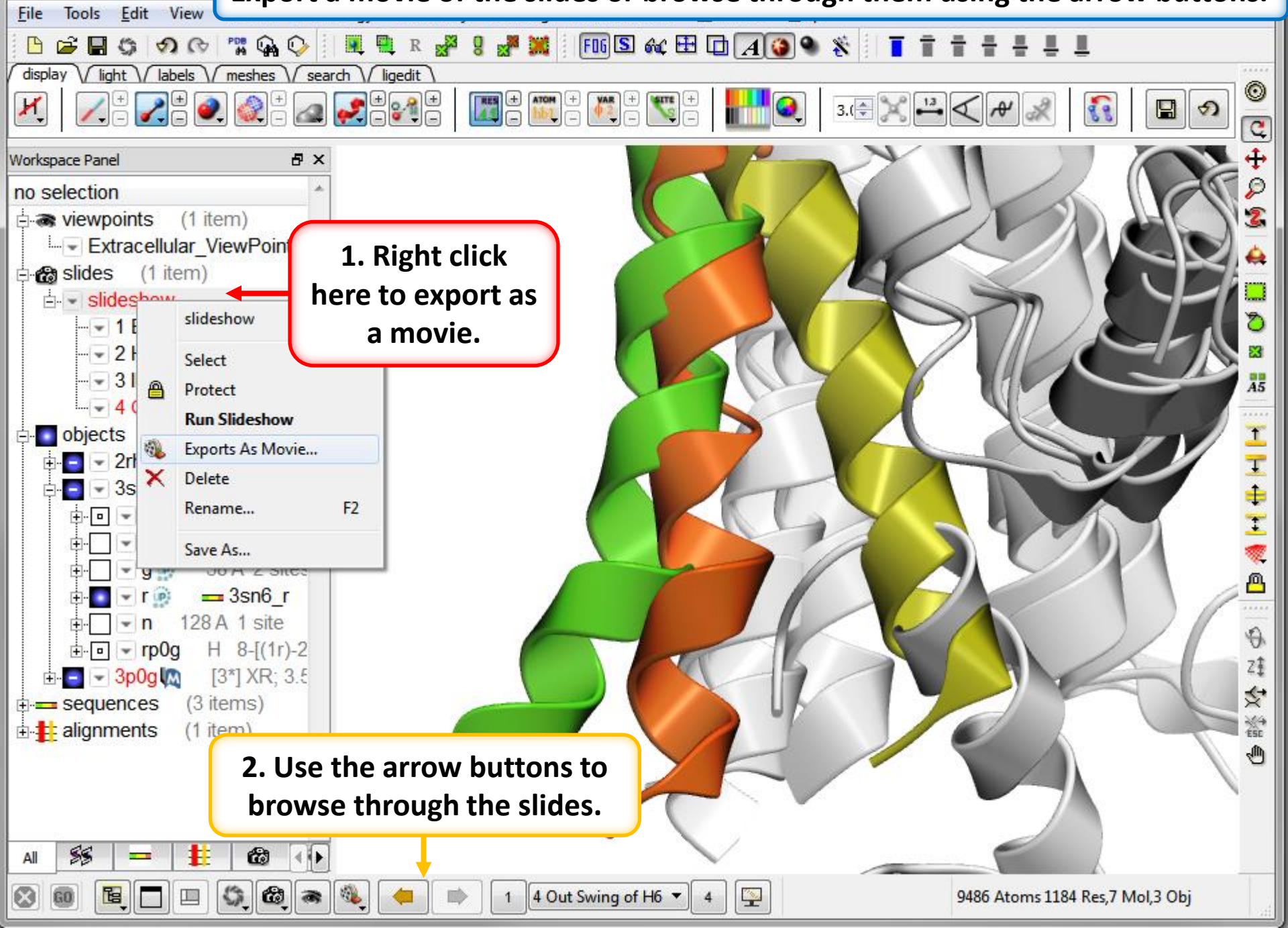
no selection

- viewpoints (1 item)
 - Extracellular_ViewPoint
- slides (1 item)
 - slideshow
 - 1 Extracellular View
 - 2 H5 Inward Shift
 - 3 Ile121 and Phe282
 - 4 Out Swing of H6
- objects (3 items)
 - 2rh1 [1] XR; 2.4Å
 - 3sn6 [2] XR; 3.2Å
 - a 349 A 4 sites
 - b 340 A 1 site
 - g 58 A 2 sites
 - r 3sn6_r
 - n 128 A 1 site
 - rp0g H 8-[(1r)-2
 - 3p0g [23] XR; 3.5Å
- sequences
- align



1. Click on the camera button to make a slide.

Export a movie of the slides or browse through them using the arrow buttons.



1. Right click here to export as a movie.

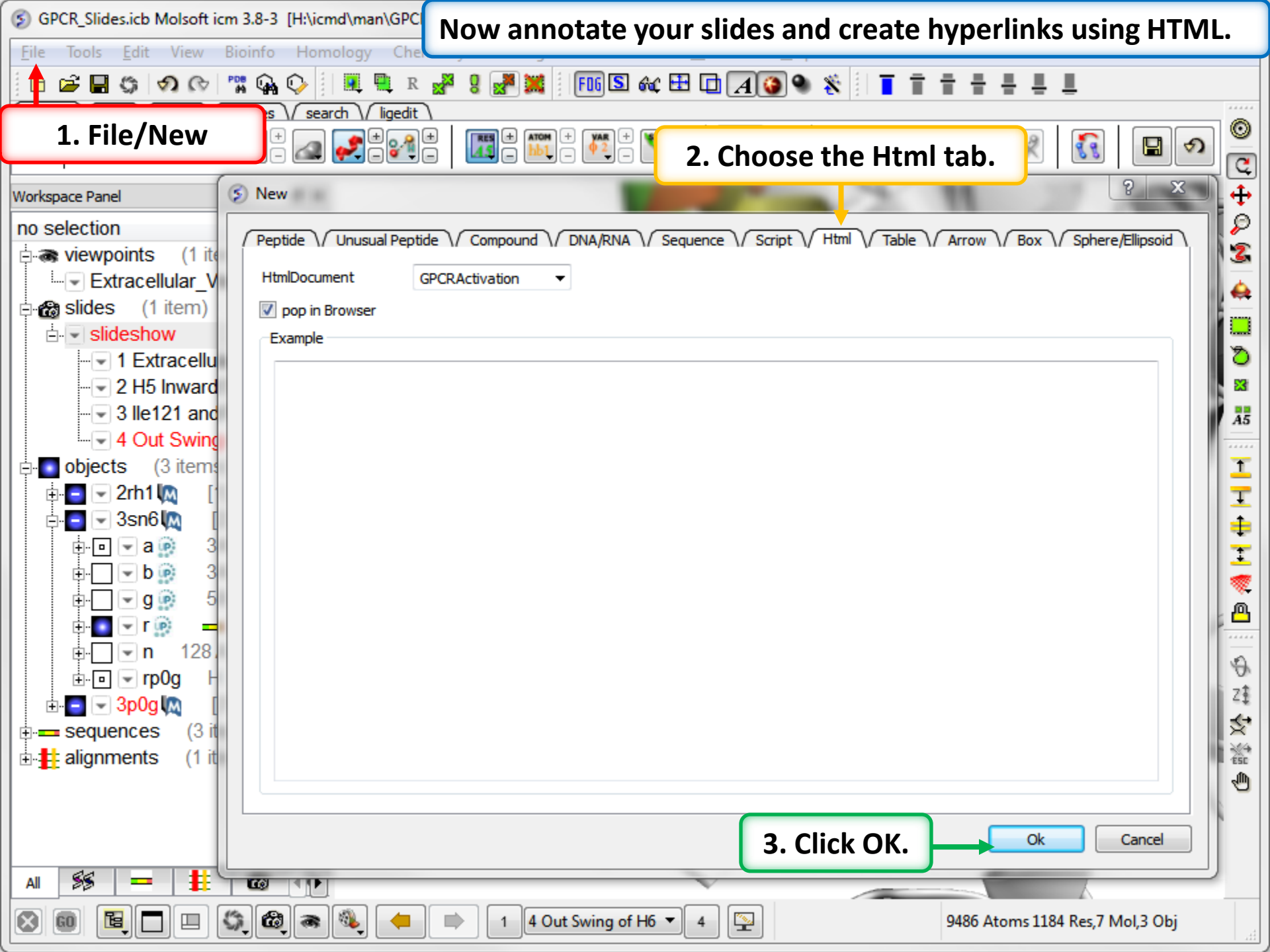
2. Use the arrow buttons to browse through the slides.

Now annotate your slides and create hyperlinks using HTML.

1. File/New

2. Choose the Html tab.

3. Click OK.



Edit the HTML document.

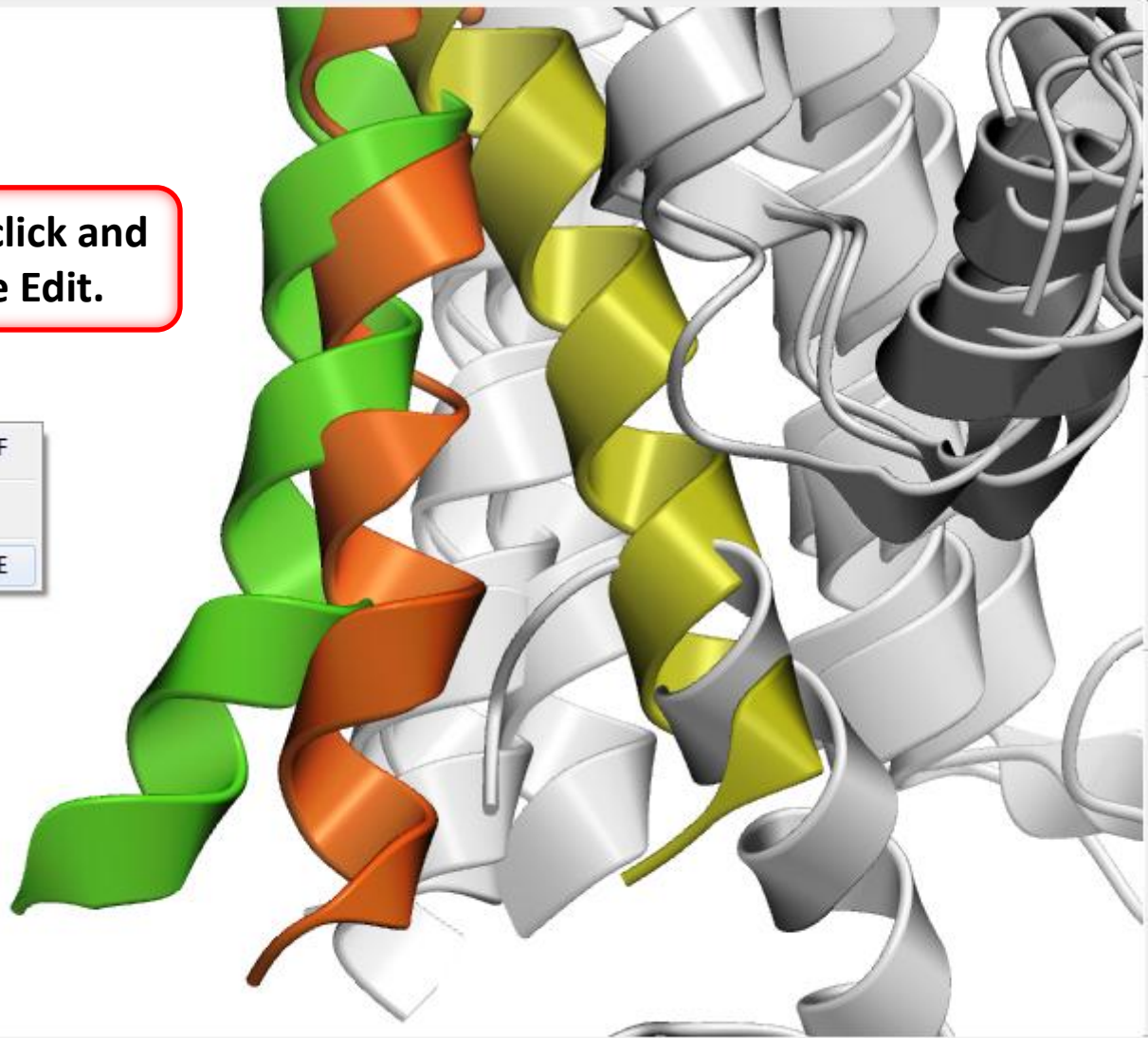
Html Documents

GPCRActivation

Workspace Panel

1. Right click and choose Edit.

- Find in Text... Ctrl+F
- Go Back
- Edit Ctrl+E**



Add some text and create hyperlinks to the slides.

File Tools Edit View Bioinfo Homology Chemistry Docking



display light labels meshes search ligedit



Html Documents

GPCRActivation

Changes Clipboard Font Paragraph

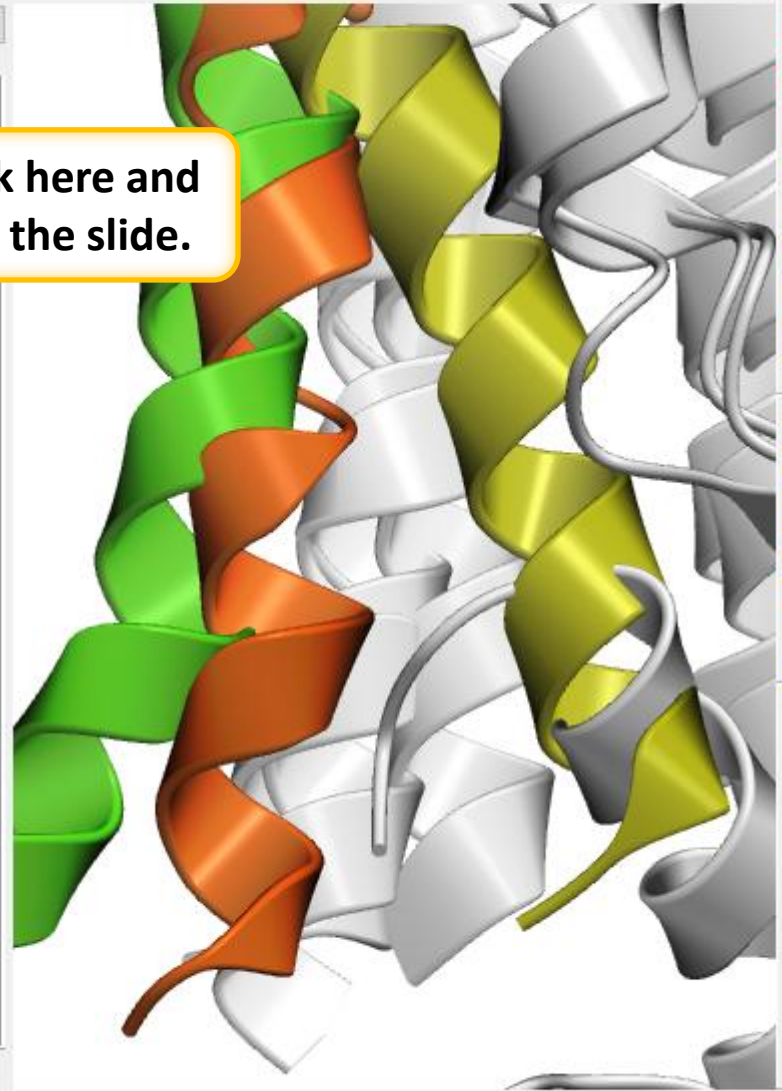
External Link Action Slide

Slide Insert

2. Click here and select the slide.

1. Select the text to make a hyperlink.

Agonists that bind to the Beta 2 Adrenergic receptor cause a conformational shift in [Helix 6](#).



View Edit Source Split

Save and Exit editing

Workspace Panel Html Documents



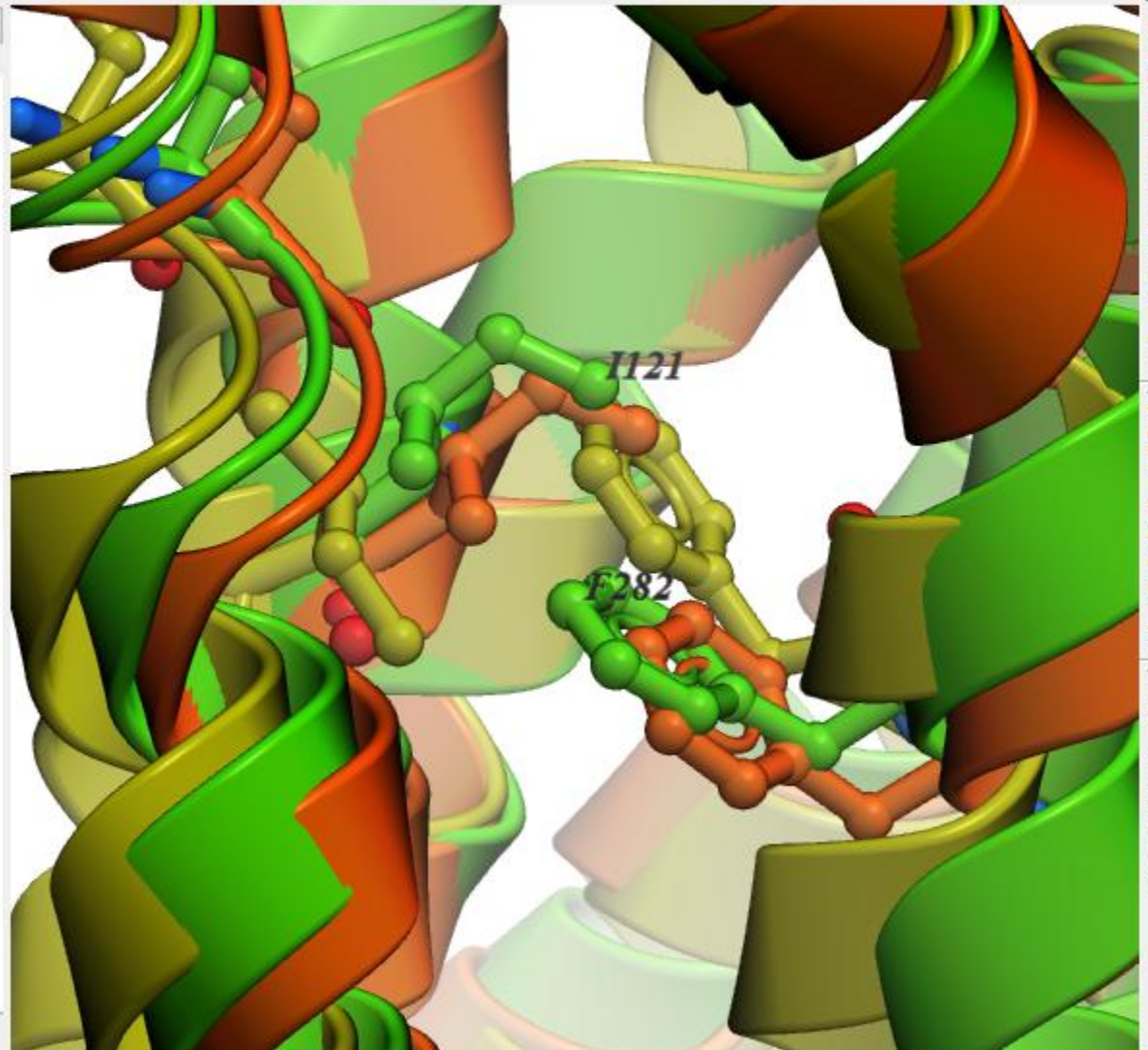
9486 Atoms 1184 Res,7 Mol,3 Obj

Save the Molecular Document as an icb file. The file can be exported to a web browser or into Windows PowerPoint.

1. File/Save As...

GPCR Activation

Agonists that bind to the Beta 2 Adrenergic receptor cause a conformational shift in [Helix 6](#). Agonists interact with [Ser203](#) and [Ser207](#) on Helix 5 which causes the extracellular section of Helix 5 to shift inwards. This results in a [rotamer change](#) of Ile121 and a movement of Phe282.



Workspace Panel Html Documents

9486 Atoms 1184 Res,7 Mol,3 Obj