Detailed Instructions for Creating an Embedded Virtual 3-D Image of a Molecule

Creating the documents with embedded virtual three-dimensional images may be done fairly easily by repeating the following procedures. Once you have embedded your first image, the use of that image is limited only by your imagination. The following instructions are written in extreme detail with annotated screen shots of the four programs you will use throughout for clarification. Once you are familiar with the procedure embedding a structure of interest should take less than 20 min., limited only by the speed with which you can click a mouse. In practice most of our embedded 3-D images have been created by our undergraduate student collaborators.

Step 1. Creating a 2-D image in ChemSketch

Using ACD ChemSketch 11.0 Freeware (http://www.acdlabs.com/download/chemsk_download.html) a two dimensional structure may be drawn as per your specific need (see Figure 1). Once the molecule is drawn, optimized it by clicking the 3-D optimization button [icon] then save as an MDL molfile (*.mol).
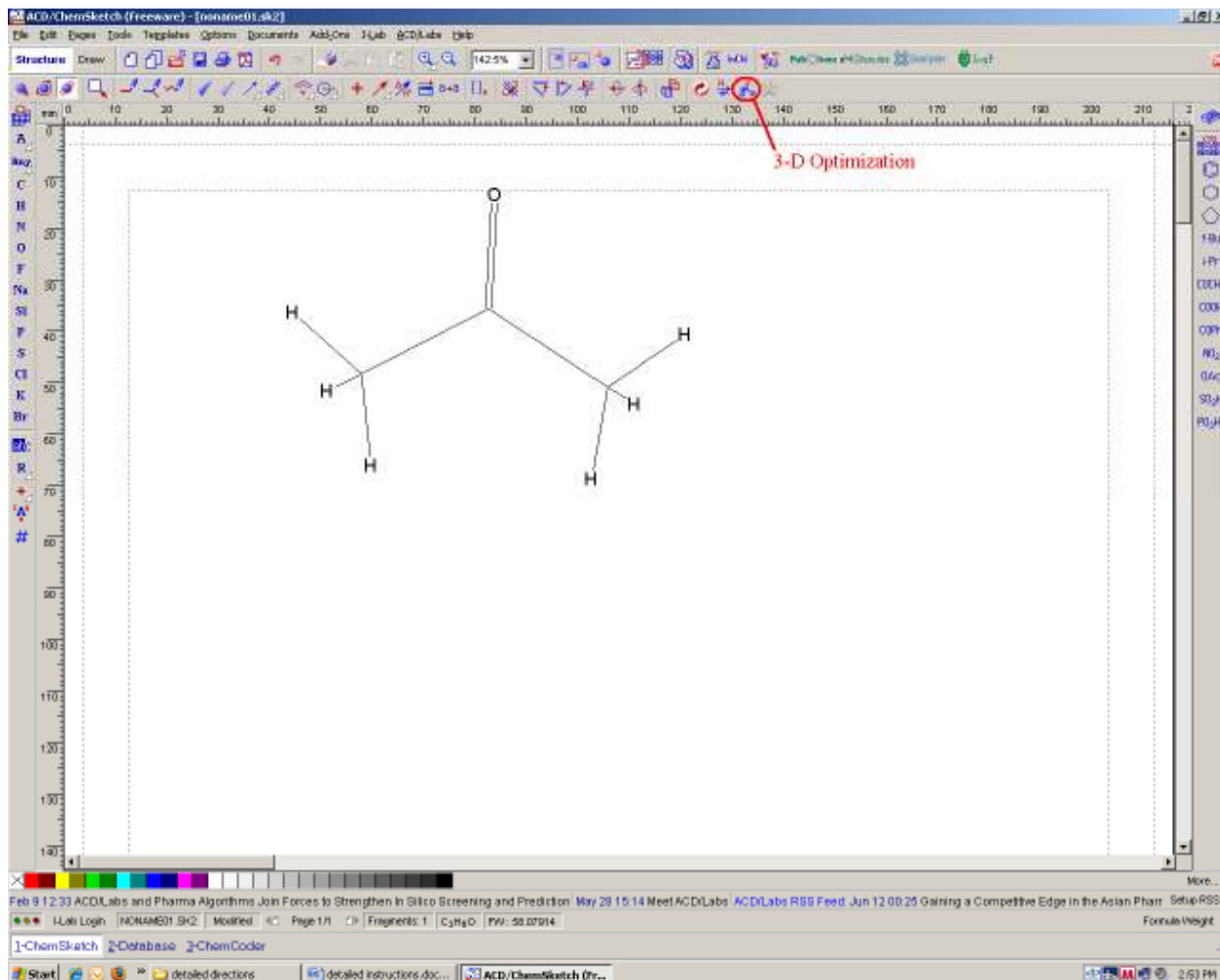

Figure 1: A screen shot of acetone drawn with ChemSketch after 3-D optimization.

Step 2. Converting the *.mol file to a *.pdb file using Open Babel

The file can now be converted from a .mol file to a .pdb file, Protein Data Bank format, to be properly accessed with the Adobe Acrobat 3D Toolkit 8.1.0. The file conversion is done using Open Babel Graphical User Interface v2.2.0 (openbabel.sourceforge.net) under default settings.

Step by step instructions:
  A. Select format of original file (see figure 2)
  B. Locate the file to be converted
  C. Select format of output file
  D. Name and provide location for output file
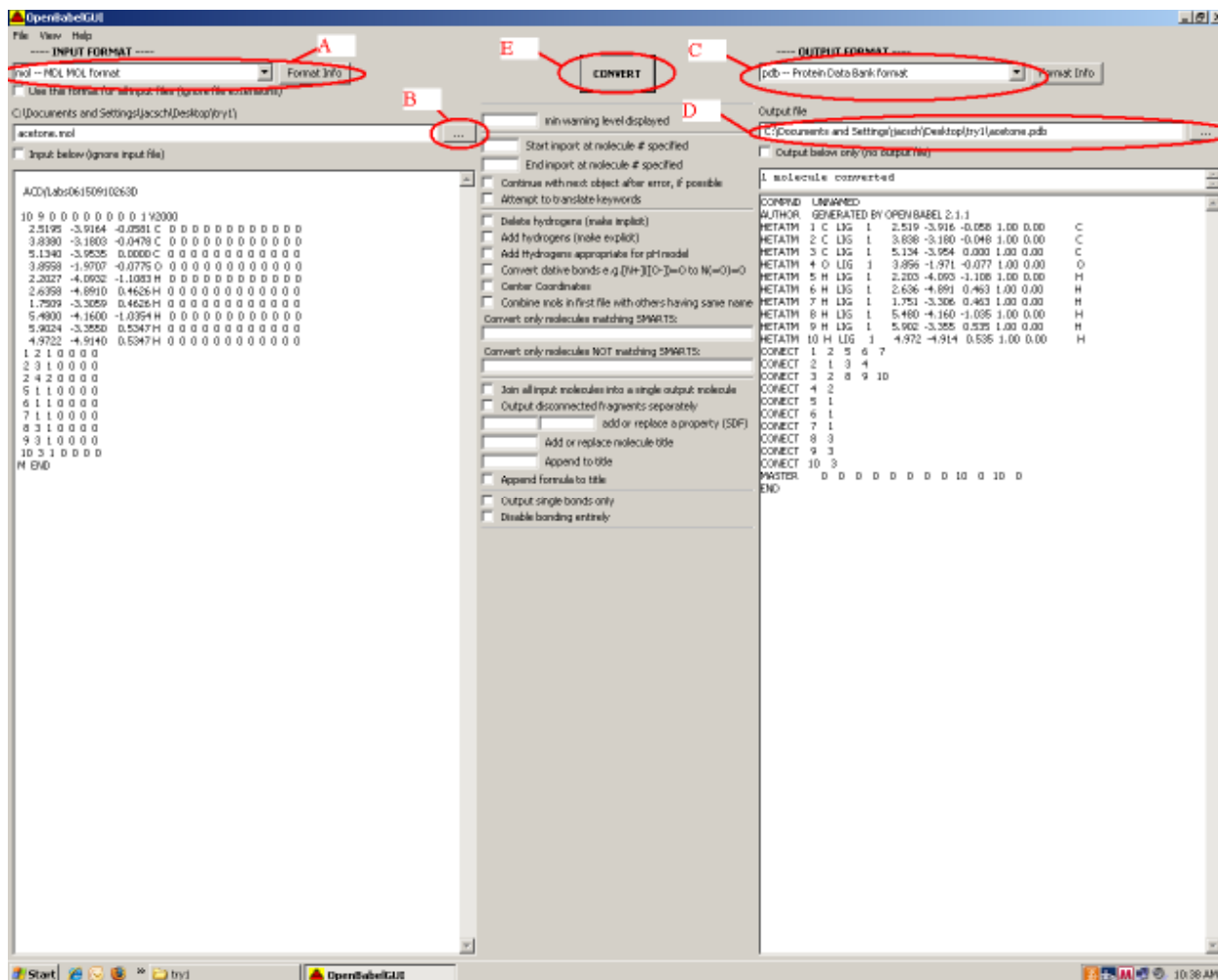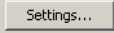 E. Click the convert button to convert file

Figure 2: A screen shot of Open Babel after conversion of the acetone.mol file to the acetone.pdb file.

Step 3. Using Acrobat 3D Toolkit to create a layered *.rh file from the *.pdb file

Once converted, the file can be opened in Adobe Acrobat 3D Toolkit changing the import settings to view as "Wire" and color "By Atom". The file is opened as the wire view of the molecule. Layers are then applied by merging the file with the same molecule only changing the import settings to "Balls and Sticks", and again separately merging the file with the "Spacefill" view. Each layer can then be accessed individually by selecting the desired layers from the Scene Tree of Toolkit. At this point any imperfections in the structures should be corrected before proceeding. By saving the file as a Right Hemisphere Binary file (*.rh), it may now be accessed and imported into Adobe Acrobat 3D.

Step by step instructions for opening a file in toolkit:

A. Open a file (see Figure 3)
B. Select the type of file -> Protein Data Bank (*.pdb) and find the *.pdb file you require
C. Click the settings button Settings... to set settings
D. Set the settings view to wire and color to by atom
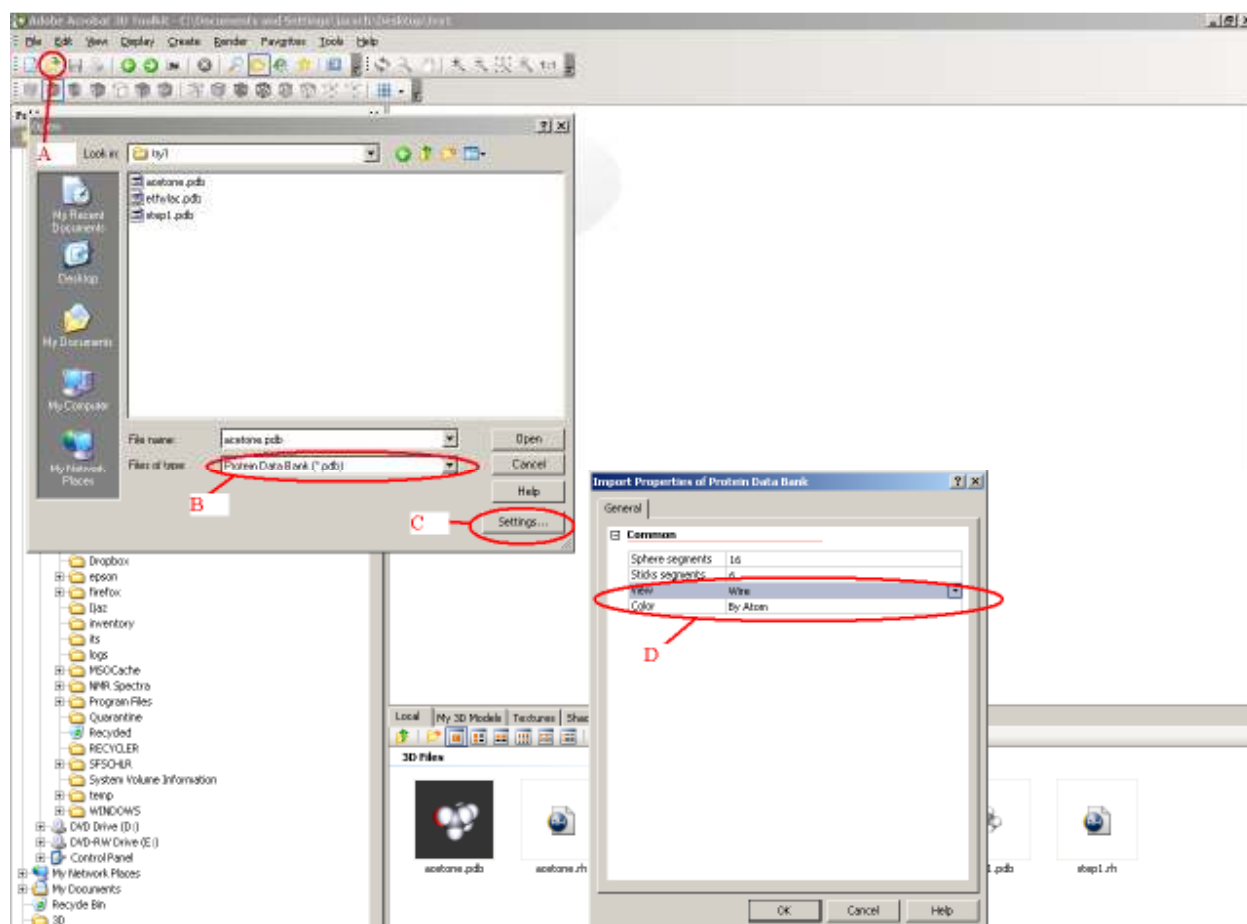E. Click OK and then click Open

Figure 3: A screen shot showing both popup windows for opening a file and adjusting the settings.

Step by step instructions for merging files (adding layers) in toolkit:
A. Click File then choose Merge file…(see Figure 4)
B. Ensure the correct file and type are selected
C. Click the settings button to set settings (do not click merge settings)
D. Set the settings view to balls and sticks and color to by atom
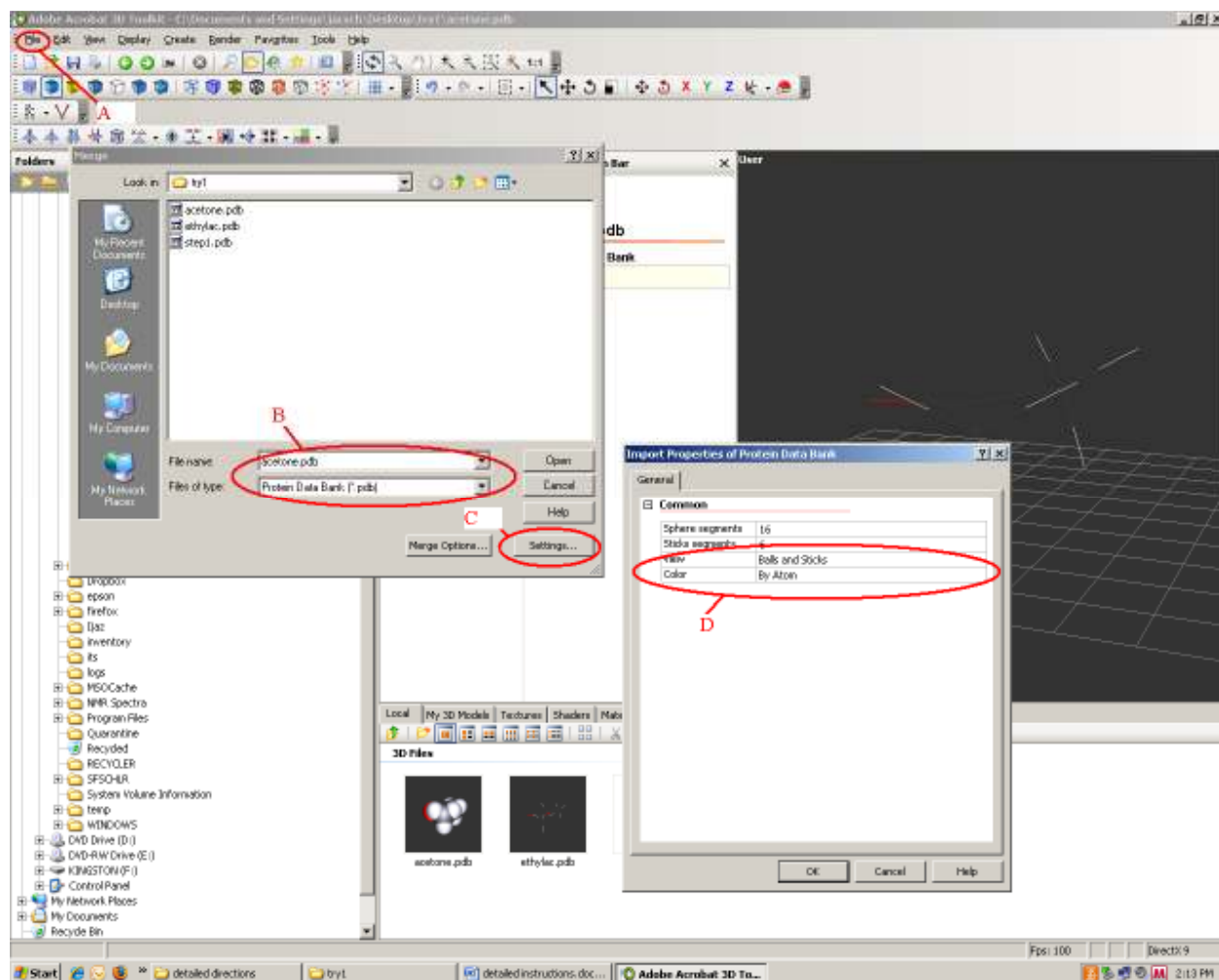E. Click OK and the click Open

Figure 4: A screen shot showing both popup windows for merging a file (balls and sticks layer) and adjusting the settings.

Step by step instructions for merging files (adding layers) in toolkit:

    A. Click File then choose Merge file…(see Figure 5)
    B. Ensure the correct file and type are selected
    C. Click the settings button to set settings (do not click merge settings)
    D. Set the settings view to spacefill and color to by atom
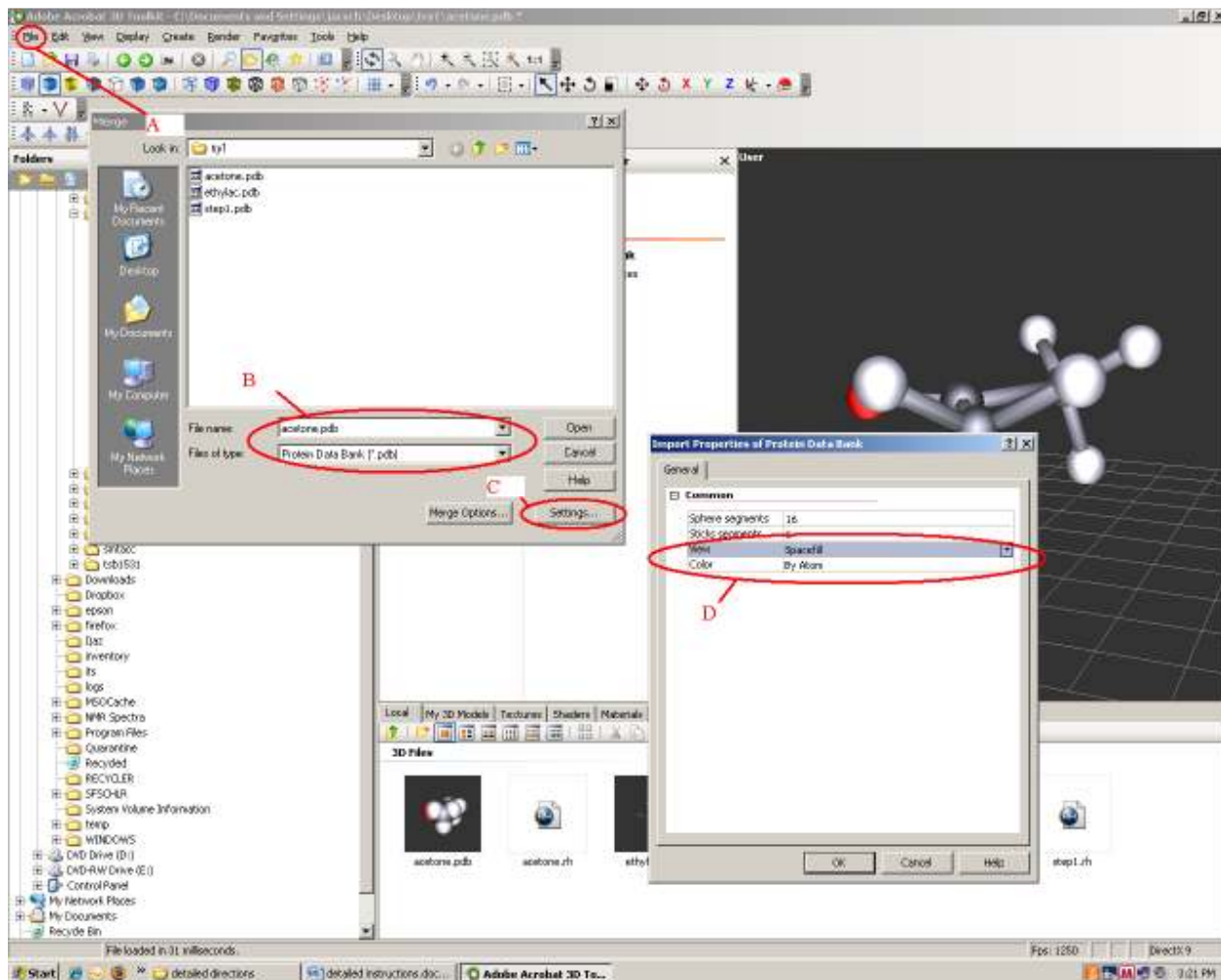   E. Click OK and then click Open

Figure 5: A screen shot showing both popup windows for merging a file (spacefill layer) and adjusting the settings.

Step 4. Design a PDF template for embedding your virtual 3-D images

A PDF template may be designed for the files using Adobe InDesign CS3 5.0.3 and exported as an Adobe PDF file.

Step 5. Embedding your virtual 3-D image into a pdf formatted document

Open created pdf file with Adobe 3D and then insert the 3D molecule using the 3D tool. Draw a box with the 3D tool for the 3D content to will open a dialogue box. Select the Right Hemisphere Binary, change the background to white, and the light to headlamp. The file will now open with all three layers.

Step by step instructions for embedding 3-D image in Acrobat 3D:
  A. Select the 3-D tool [icon] and create a box to put 3-D image in by left mouse hold and drag on document (see Figure 6). A pop up window appears.
  B. Open the right hemisphere file (*.rh) you created in toolkit
  C. Set the background color to white
  D. Set the lighting to headlamp
  E. Click OK and another pop up box opens. Select OK again and your image will be inserted (see Figure 7).
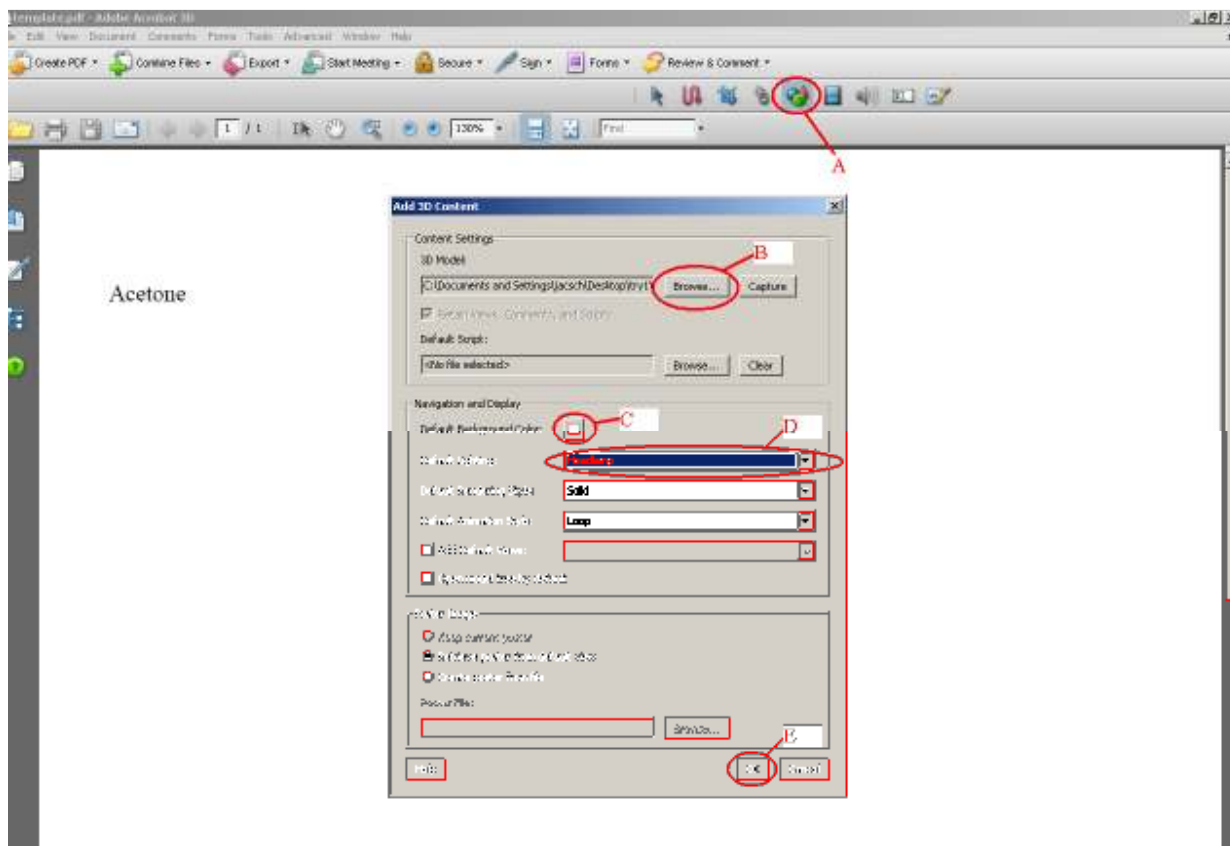

Figure 6: A screen shot of the setting dialogue box for inserting you image.
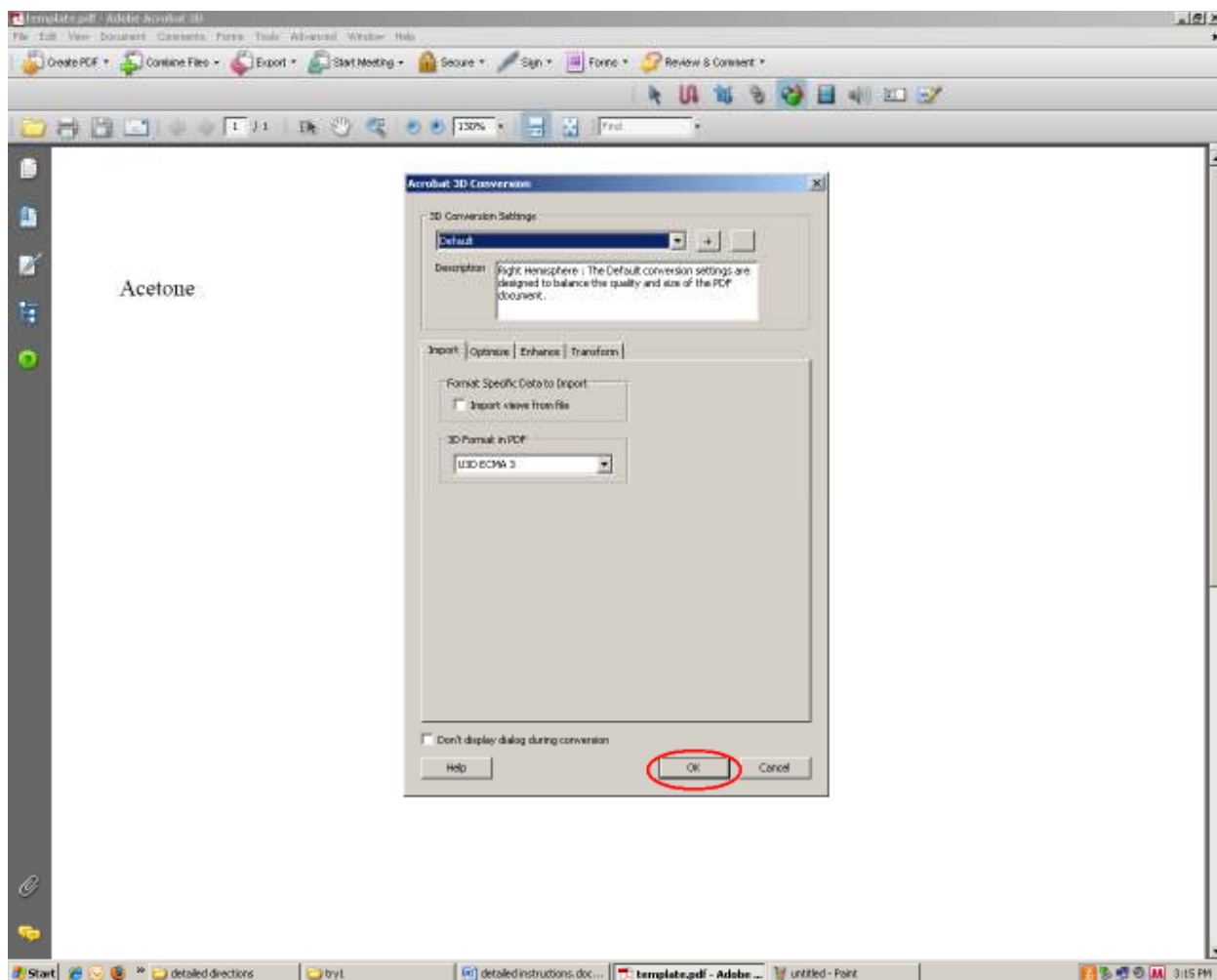
Figure 7: A screen shot of the second popup box that appears after completing the settings.

Step 6. Installing the dropdown buttons to toggle between structure views

Buttons may be inserted to control the exchange between the views (wire, ball and stick, and spacefill) by selecting the structure to be controlled with the select tool, opening the model tree, checking the boxes to display the desired layer, and taking a snapshot of the layer in the desired position using the camera tool.

Step by step instructions for opening the model tree

A. Select the hand tool 🖐 (see Figure 8)
B. Using the hand tool click on the structure to activate the virtual 3-D image

C. Click on model tree button 🔳 to open the model tree (see Figure 9)
D. The model tree will be used to create buttons for the virtual 3-D image to navigate between the wire, ball and stick, and spacefill structures.
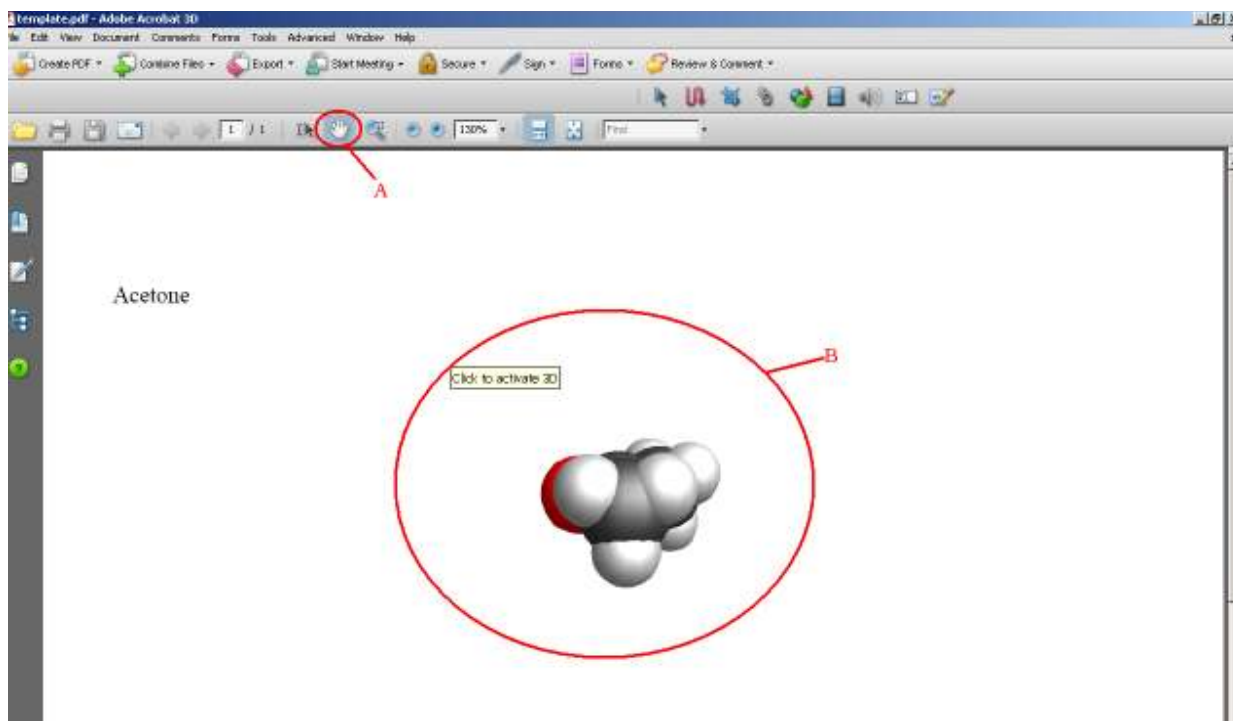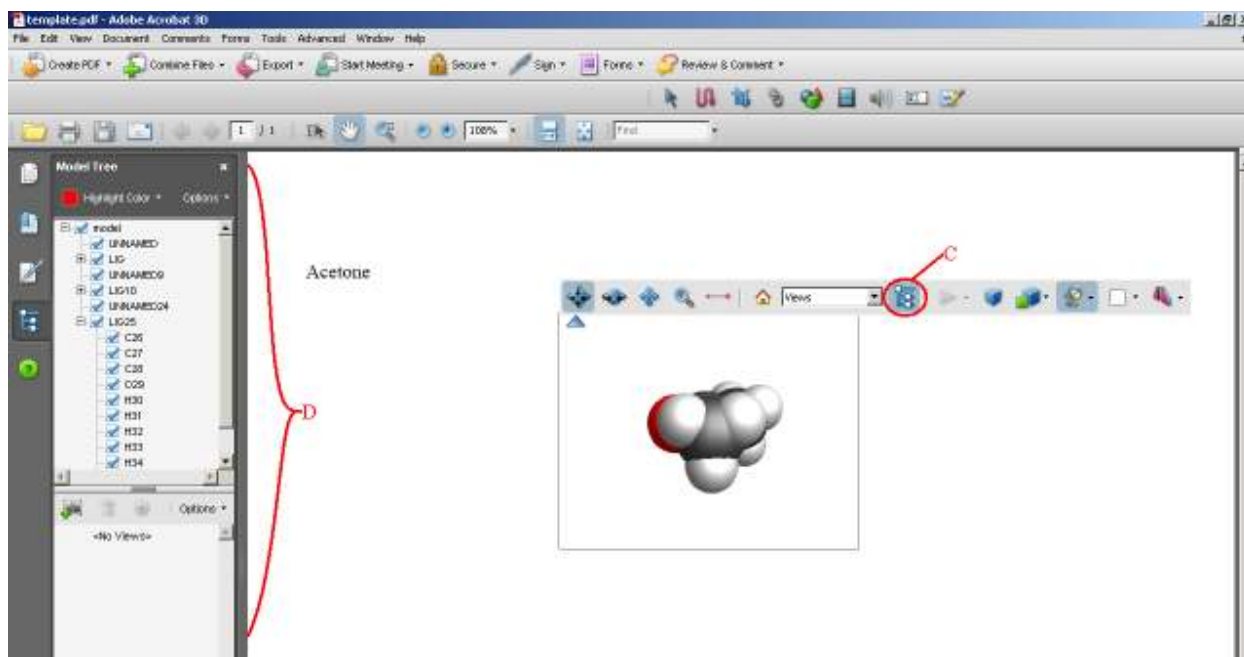
Figure 8: A screen shot showing the hand tool and structure.

Figure 9: A screen shot after the Model Tree is opened.

Step by step instructions for using the model tree to add buttons to view the different models (wire, ball and stick, and spacefill):

A. Deselect the ball and stick and spacefill views on the model tree (see Figure 10)

B. Click the create view button

C. Rename the newly created view by clicking on the name and type in wire

D. Notice when you now place your mouse over the structure the wire view is available in the drop down menu

E. Deselect the wire view and select the ball and stick view (see Figure 11)

F. Click the create view button

G. Rename the newly created view by clicking on the name and type in ball and stick

H. Notice when you now place your mouse over the structure the ball and stick view is available in the drop down menu

I. Deselect the ball and stick view and select spacefill view (see Figure 12)

J. Click the create view button

K. Rename the newly created view by clicking on the name and type in spacefill

L. Notice when you now place your mouse over the structure the spacefill view is available in the drop down menu
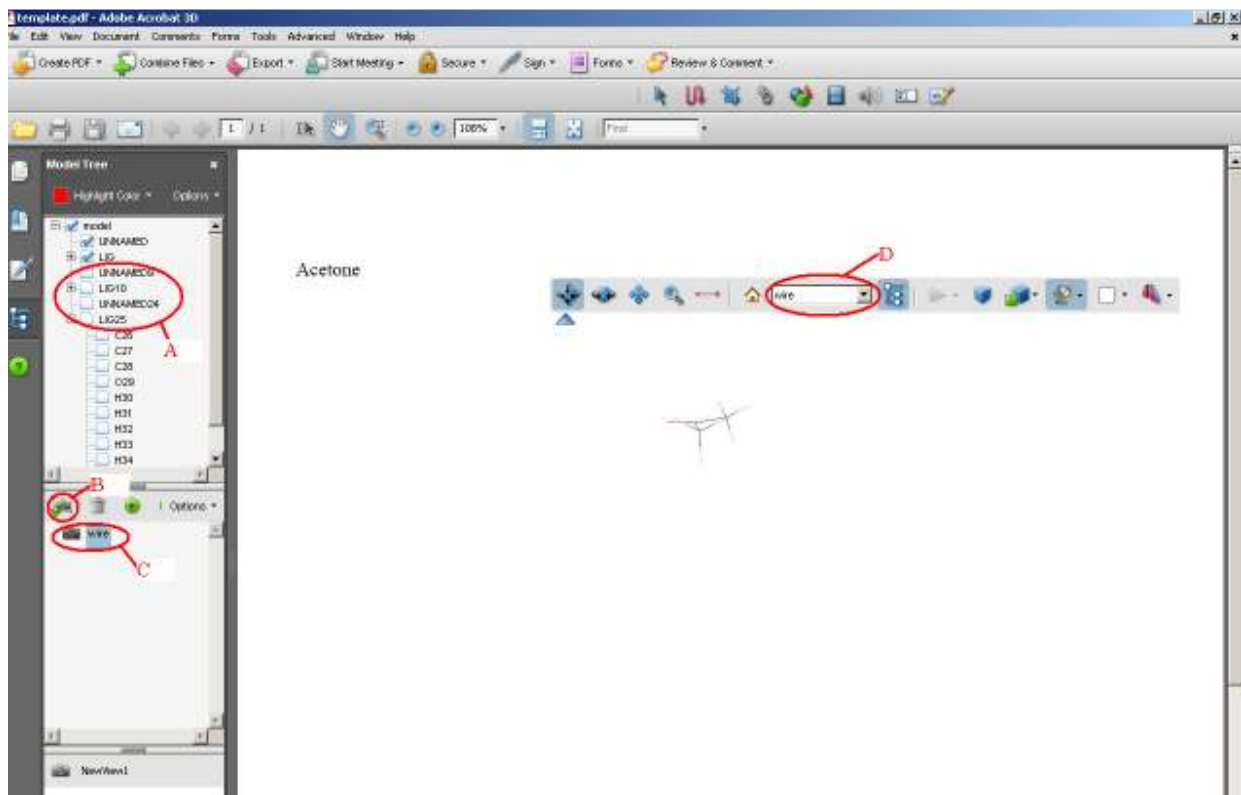

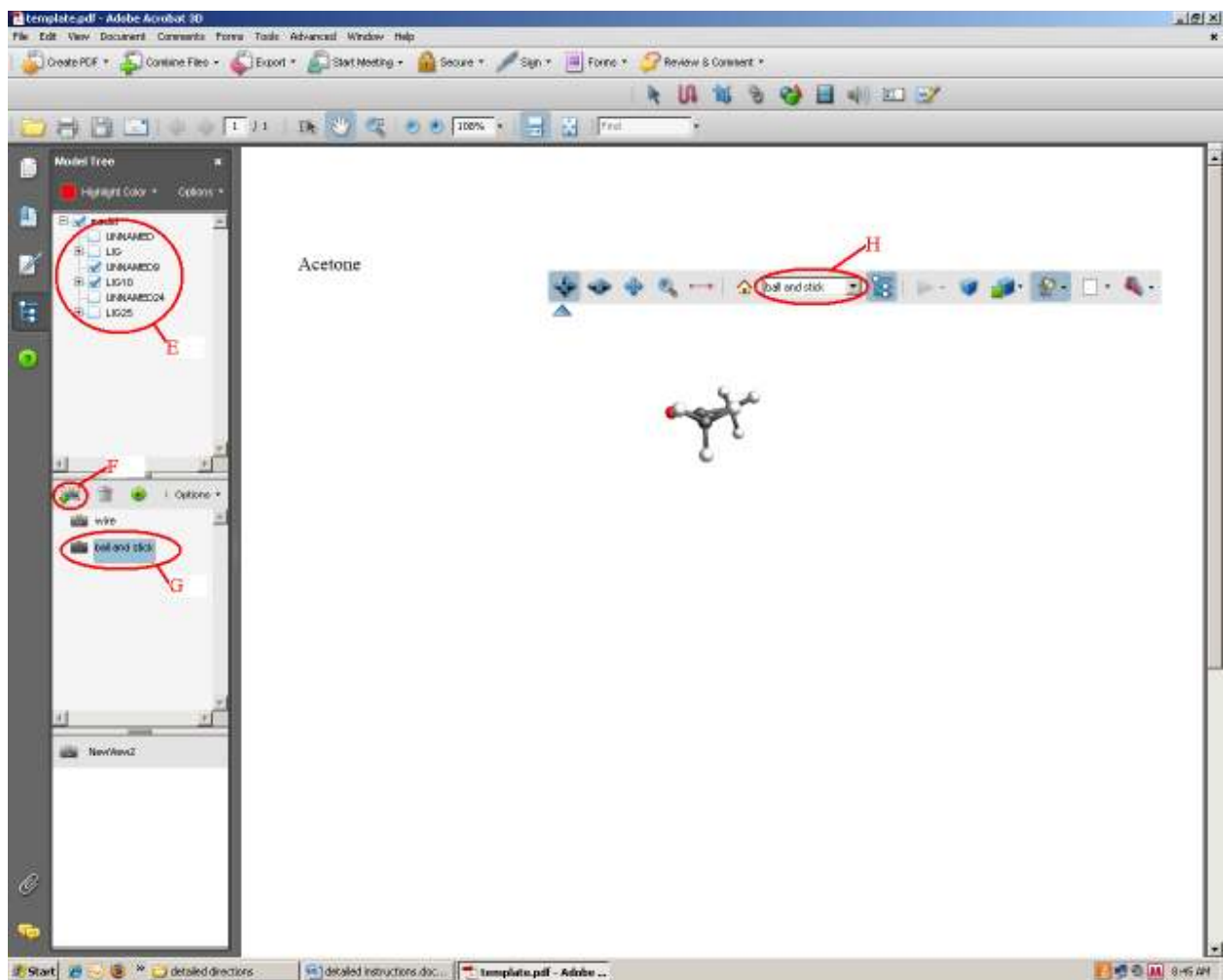Figure 10: Screen shot of wire tab creation.

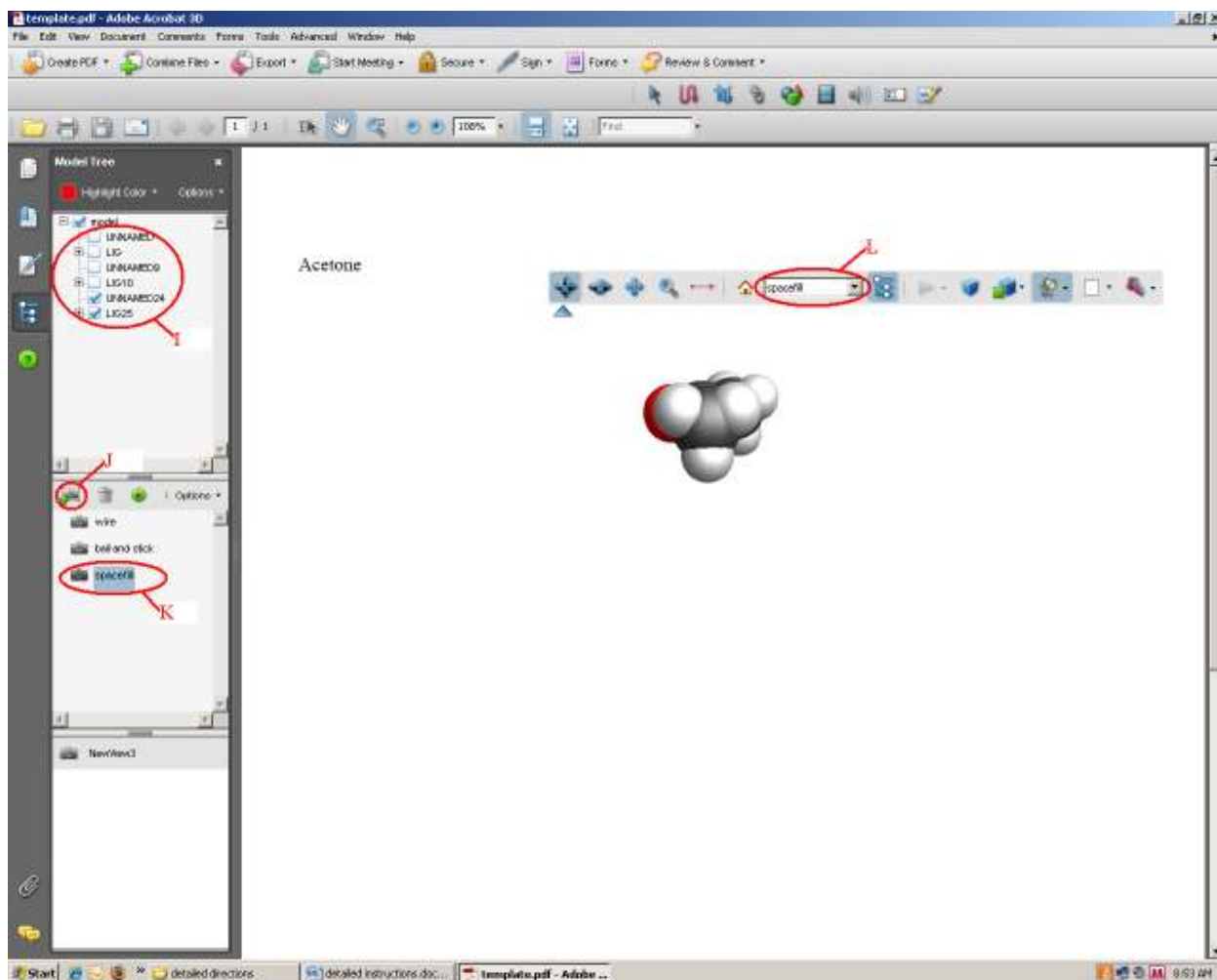Figure 11: Screen shot of balls and sticks tab creation.

Figure 12: Screen shot of spacefill tab creation

The model tree may now be closed. You have created an embedded virtual 3-D image of a molecular structure.