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# MOLECULAR VISUALIZATION

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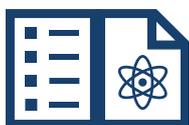
## Learning goals of the activity:

- Familiarize with computational visualizations of molecules.
- Acquire skills in drawing molecules and studying 3-dimensional representations.
- Introductory understanding of structural properties of molecules.
- Use search functions to find and visualize known molecules.

## Building and visualizing small molecules

Open <https://molview.org/>

1. We begin by looking at the Information card for the molecule already shown in the program. This can be found in the menu, under "Tools".
  - a. Fill in the first row of the table below with details of this molecule (next to "a"), using its information card.
  - b. Use the search function in the top left corner to load the molecule *Acetaminophen*, and open its information card.  
Fill out the second row of the table below with details of this molecule (next to "b").



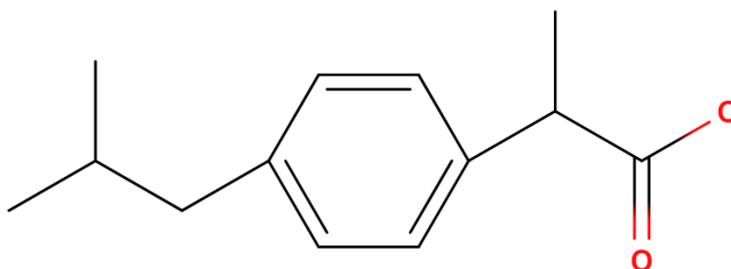
Name	Type of molecule (written in the text description)	Weight of molecule	Percentage of molecular weight that is oxygen
a.			
b. Acetaminophen, or:  _____ (its more common name).			

Weights of molecules are commonly given in the unit "u"; numbers followed by "u" will indicate molecular weights (eg. "151.16 u").

2. Clear the drawing board using the button:



- a. Using the drawing tools, draw the following molecule:



- b. What is the name of this molecule according to its information card?

- c. Click the "2D to 3D" button and study the 3D-image of the molecule.

The lines and wedges on the top left of the screen are used to draw atomic bonds.

The rings and line below are used to add carbon chains and (cyclic) rings.

At the top you also find the eraser, undo button, *move* and *selection* tools:



The letters in the middle (C, H, N, O, P etc.) allow you to add atoms by clicking one of them and then where you want to add it.

The left mouse button is used to rotate the 3D image of the molecule.

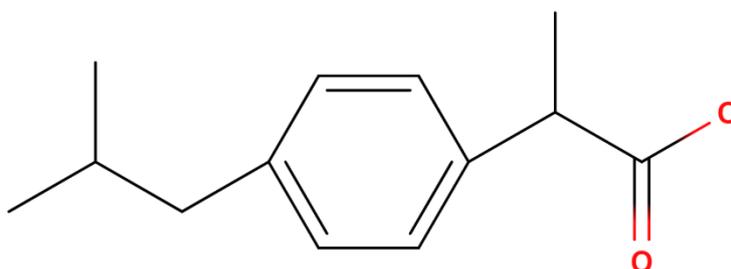
Rotating the mouse wheel zooms the image in and out.

Clicking and holding the mouse wheel lets you move the molecule sideways.

- d. Are there more atoms now that were not shown in the 2D image? If so, where are these

atoms? \_\_\_\_\_

- e. Draw them at the corresponding positions in this picture:



- f. Use the "MEP surface opaque" function to visualize the distribution of charges over the molecule.
  - g. Where is the molecule more positively charged according to this surface? What atom types does this charge correspond to?
  - h. Use the "Charges" function to examine how atomic charge values correspond to each color on the surface (reply below which respective color you see on the surface):
    - i. Negative charges show as:
    - ii. No charges ("0.0000") show as:
    - iii. Positive charges show as:
3. Find out which class this drug belongs to by using the "PubChem source" feature.
4. Which other compounds is this molecule similar to? (the "≈ similarity" function)
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