

# **Visualización y representación de estructuras cristalinas y macromoléculas**

**2º Workshop de Resolución Estructural Mediante  
Rayos-X de Monocristal**

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*Universidad Rey Juan Carlos*

## **Visualización molecular. Mercury y RasMol**

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- Los programas de visualización molecular permiten a los usuarios:
  - Rotar toda la imagen en tres dimensiones para ver las partes que no se pueden visualizar en una representación bidimensional y ver así la forma de la molécula (lo que a su vez determina su función);
  - Activar o desactivar la rotación de ciertas partes de la representación visual para ver distintas cadenas, sub-unidades y tipos de sub-moléculas; y
  - Medir ángulos y distancias de enlace dentro de la estructura. Las medidas de ángulos indican la forma de la molécula y si ella tiene en su interior enlaces sencillos, dobles, triples, etc

## **Visualización molecular. Mercury y RasMol**

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- Además, la visualización molecular no solo favorece el aprendizaje y la enseñanza, sino también puede ser un buen modelo de representación gráfica para determinadas macromoléculas como:
  - Proteínas
  - Vitaminas
  - Ácidos grasos y lípidos
  - Hidratos de carbono de cadena larga
  - ADN y otras macromoléculas de interés biológico

## **Visualización molecular. Mercury y RasMol**

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- Existen numerosos programas que permiten la visualización molecular ya sea de moléculas pequeñas, como de moléculas muy grandes. Aunque los más usados pueden ser:
  - Mercury
  - RasMol
  - ORTEP
  - Diamond
  - ViewerLite

# Visualización molecular. Mercury y RasMol

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- Mercury

- Es un programa de visualización
- Gratuito (CCDC Cambridge Crystallographic Data Centre)
- Muy interesante para moléculas pequeñas
- Especial para estructuras cristalinas

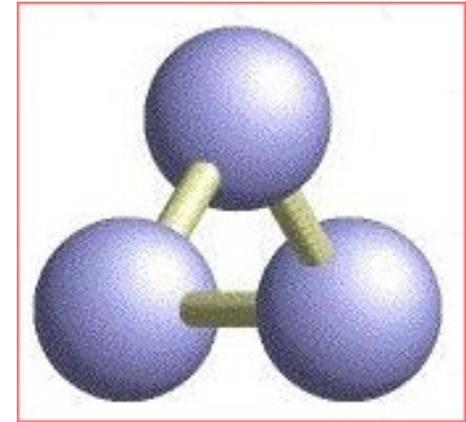


# Visualización molecular. Mercury y RasMol

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- RasMol

- Es un programa de visualización
- Gratuito (Roger Sayle)
- Muy interesante para macromoléculas
- Especial para estructuras cristalinas de proteínas que se ven muy mal en Mercury



# Visualización molecular. Mercury y RasMol

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- ORTEP

- Programa de visualización
- Gratuito (Louis Farrugia)
- Muy interesante para moléculas pequeñas
- Especial para estructuras cristalinas, es el que se usa en publicaciones científicas



# Visualización molecular. Mercury y RasMol

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- Diamond

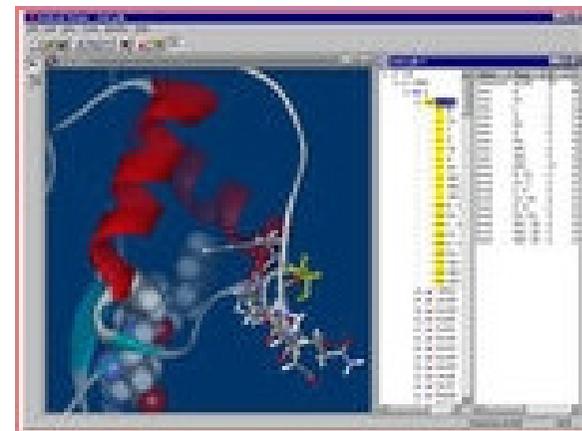
- Programa de visualización
- Con Licencia (Crystal Impact)
- Muy interesante para moléculas pequeñas
- Especial para estructuras cristalinas
- Muy complicado de utilizar



# Visualización molecular. Mercury y RasMol

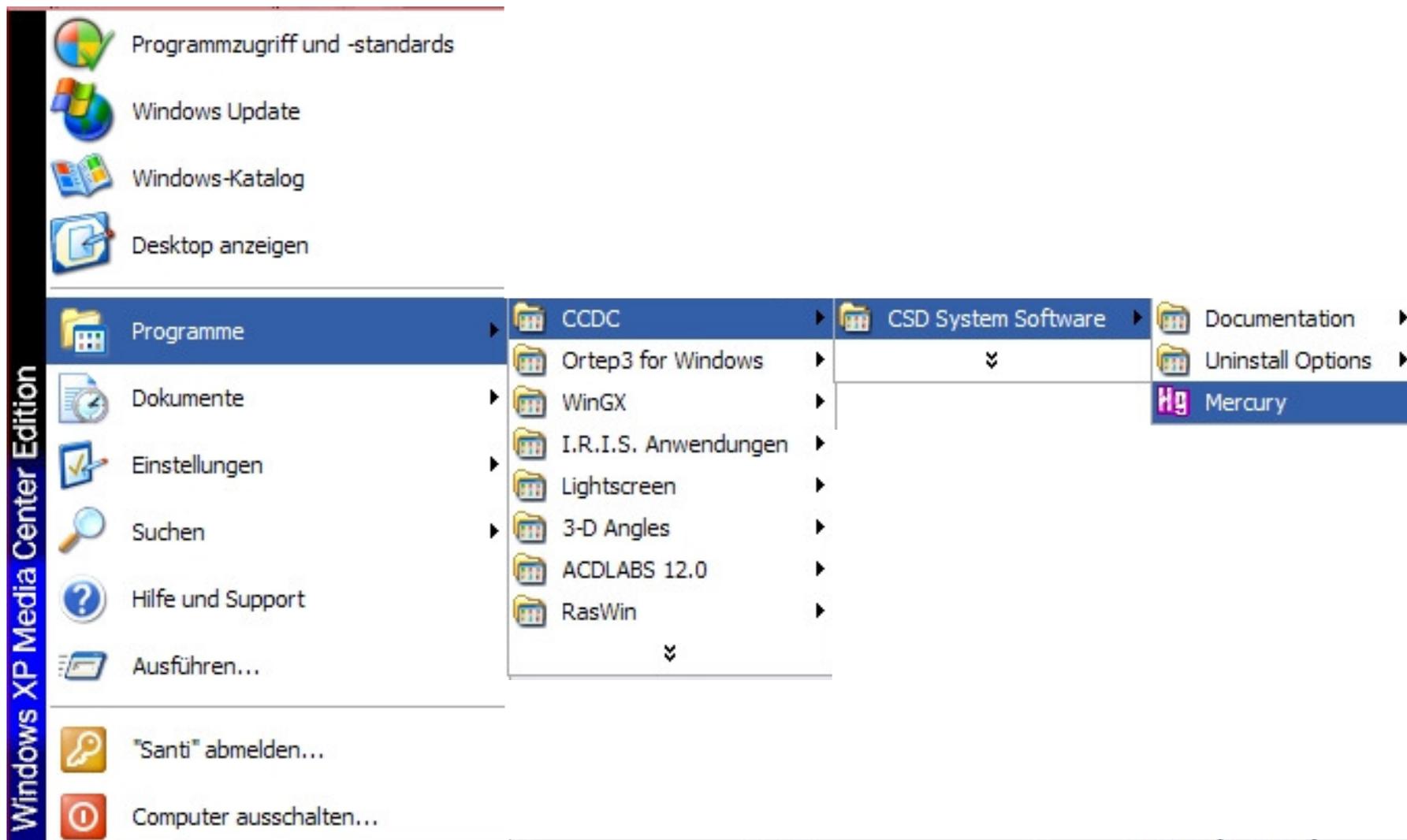
- ViewerLite

- Programa de visualización
- Sin Licencia (WebLab)
- Muy interesante para moléculas pequeñas
- Especial para estructuras cristalinas



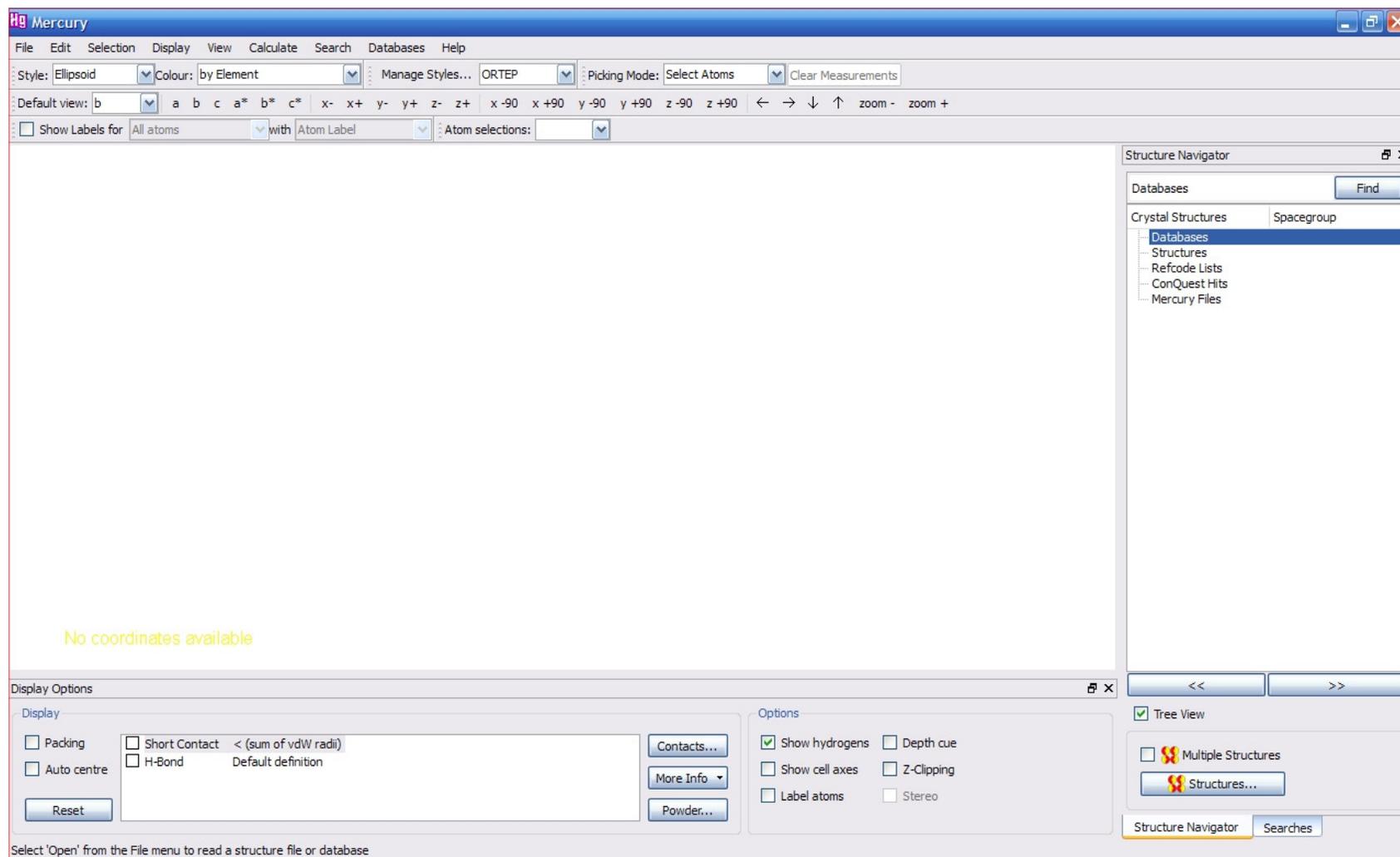
# Visualización molecular. Mercury y RasMol

- Mercury



# Visualización molecular. Mercury y RasMol

- Mercury



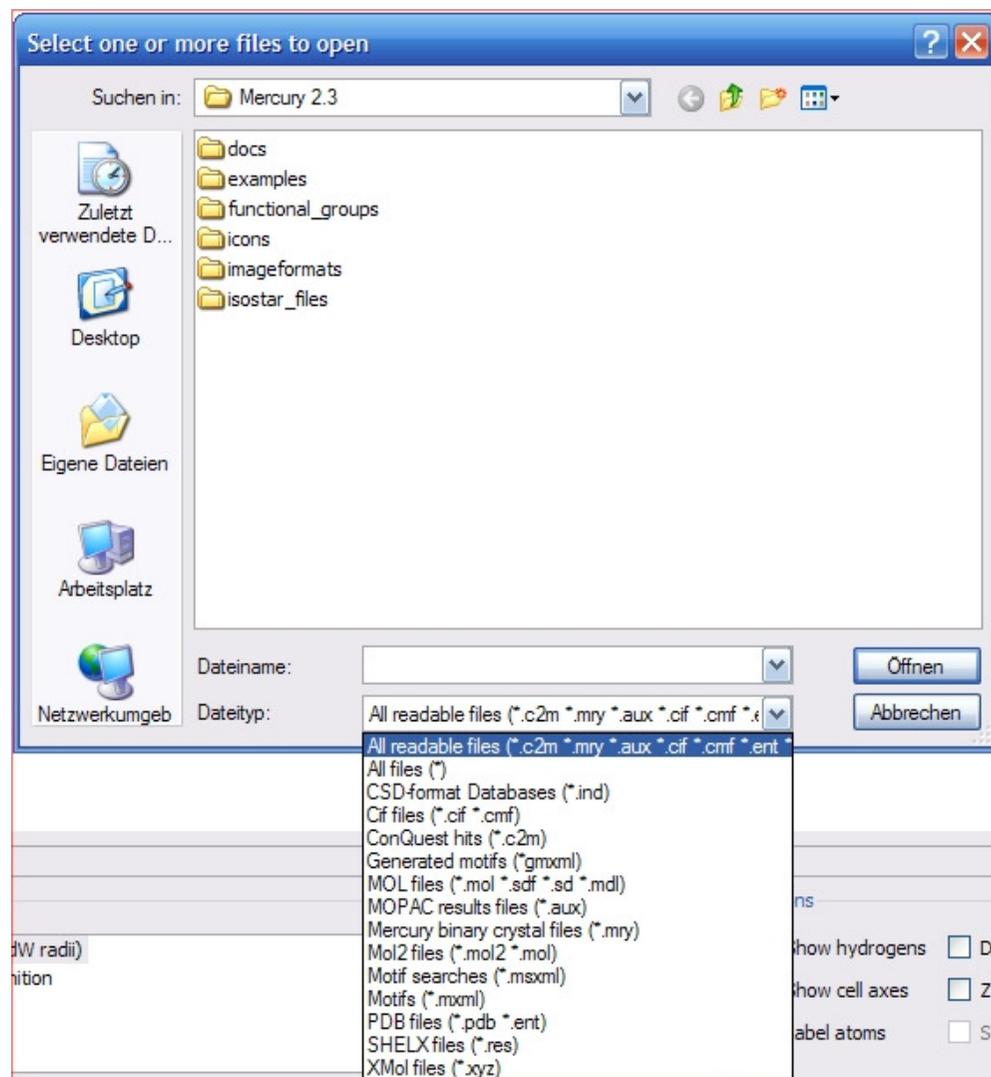
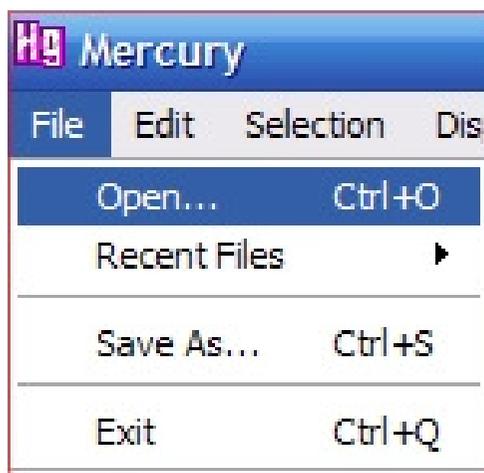
# Visualización molecular. Mercury y RasMol

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- Mercury
  - Mercury lee archivos de varios tipos
    - Archivos con información cristalográfica .RES, .CIF
    - Archivos de posiciones espaciales .XYZ,
    - Archivos de base de datos cristalográficos .IND
    - Archivos generados por ChemSketch (extension .MOL, .MOL2)
    - Archivos de Protein Data Bank (.PDB)

# Visualización molecular. Mercury y RasMol

- Mercury. Abrir Archivo

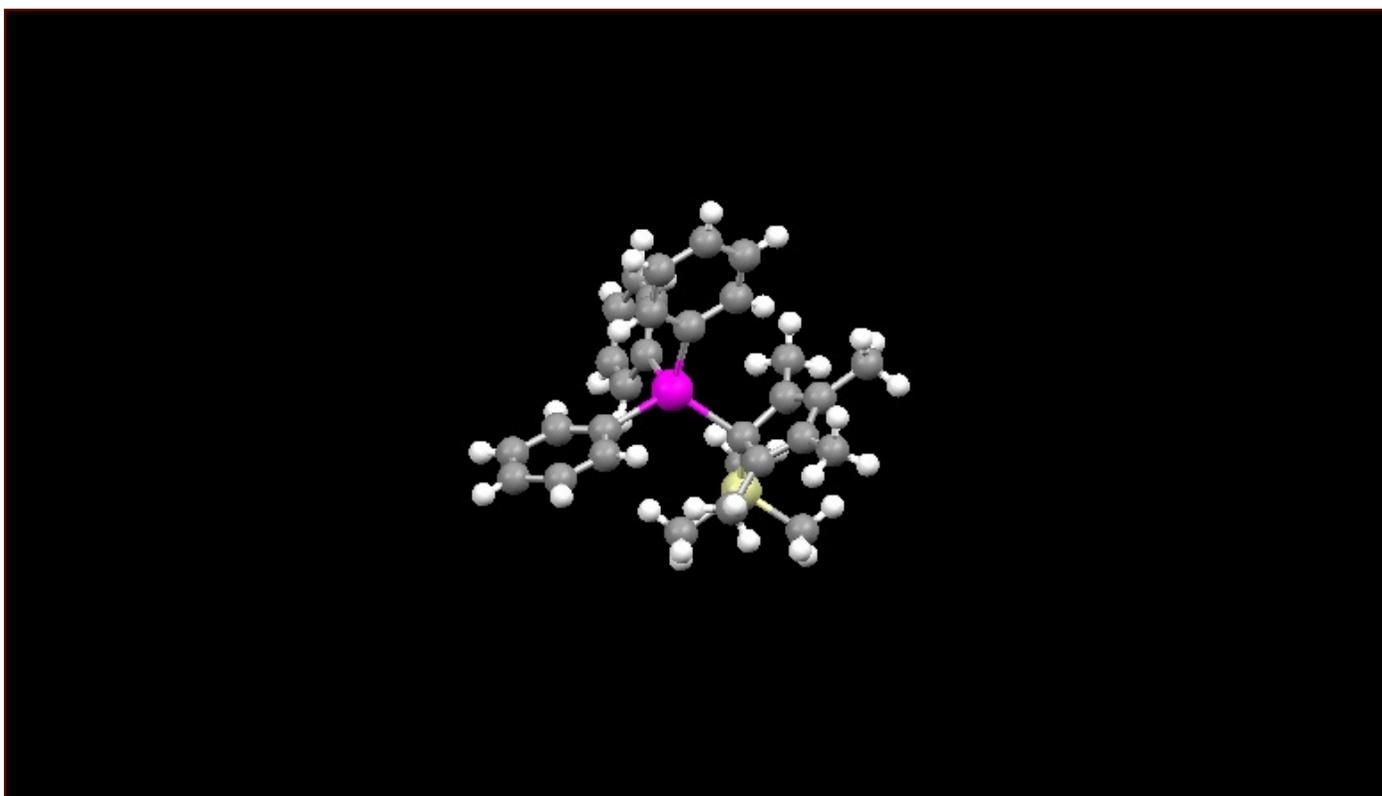
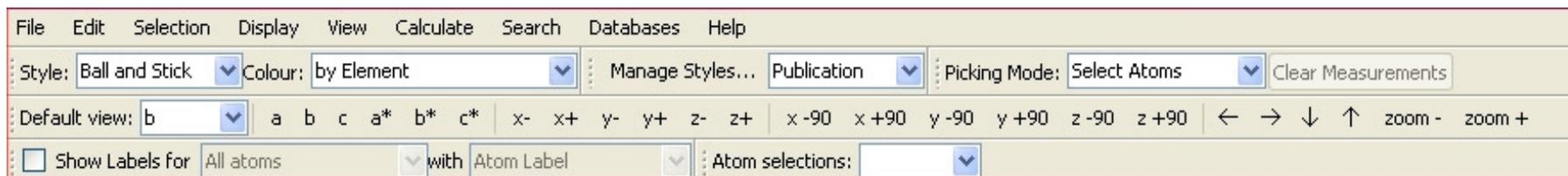


# Visualización molecular. Mercury y RasMol

- Mercury. Abrir “Estructura 1.res”

The screenshot displays the Mercury software interface. The main window shows a ball-and-stick model of a complex organic molecule with a central pink atom. The interface includes a menu bar (File, Edit, Selection, Display, View, Calculate, Search, Databases, Help) and a toolbar with various options like Style (Ball and Stick), Colour (by Element), and Picking Mode (Select Atoms). The Structure Navigator panel on the right shows a tree view of the loaded structure, with 'Estructura 1.res' selected. The Display Options panel at the bottom provides settings for display (Packing, Auto centre, Short Contact, H-Bond) and options (Show hydrogens, Show cell axes, Label atoms, Depth cue, Z-Clipping, Stereo). A note at the bottom of the interface reads: 'Press the left mouse button and move the mouse to rotate the structure'.

# Visualización molecular. Mercury y RasMol



# Visualización molecular. Mercury y RasMol

Display Options

Display

Packing

Auto centre

Short Contact < (sum of vdW radii)

H-Bond Default definition

Reset

Contacts...

More Info

Powder...

Options

Show hydrogens

Show cell axes

Label atoms

Depth cue

Z-Clipping

Stereo

Press the left mouse button and move the mouse to rotate the structure

Structure Navigator

x0674fin in P-1 Find

Crystal Structures Spacegroup

Databases

Structures

Estructura 1.res

x0674fin in... P-1

Refcode Lists

ConQuest Hits

Mercury Files

<< >>

Tree View

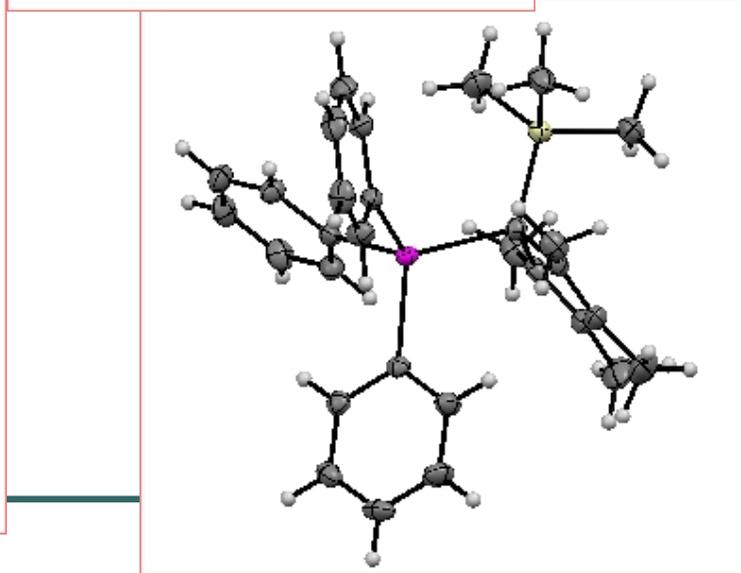
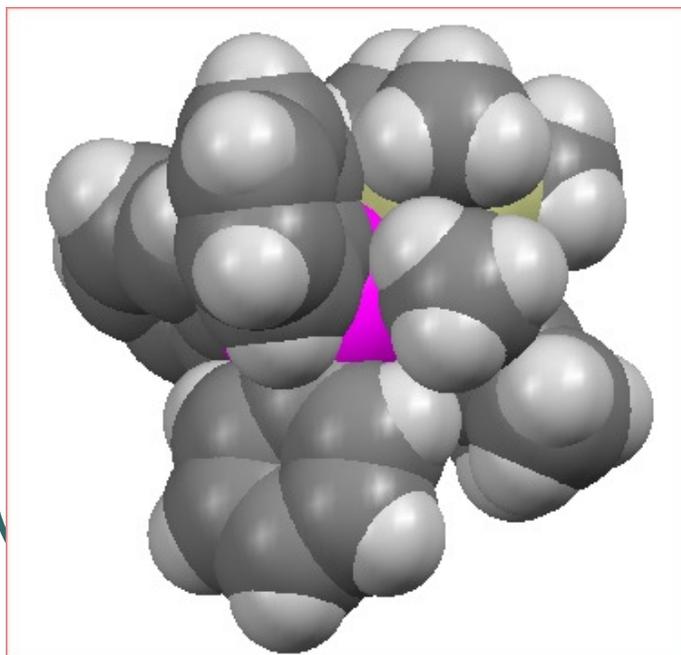
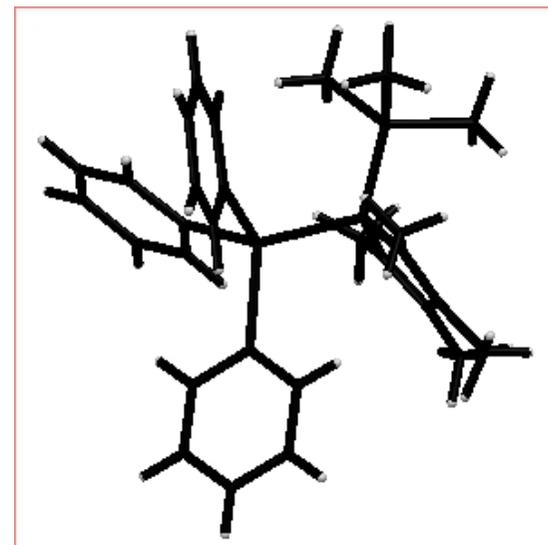
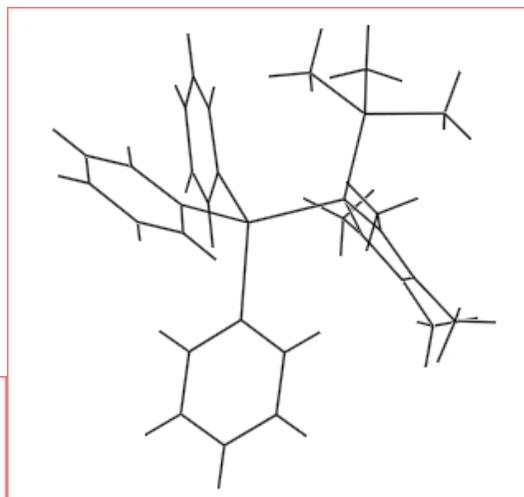
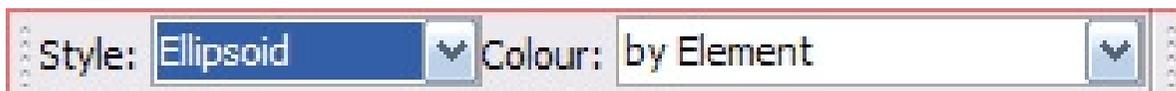
Multiple Structures

Structures...

Structure Navigator Searches

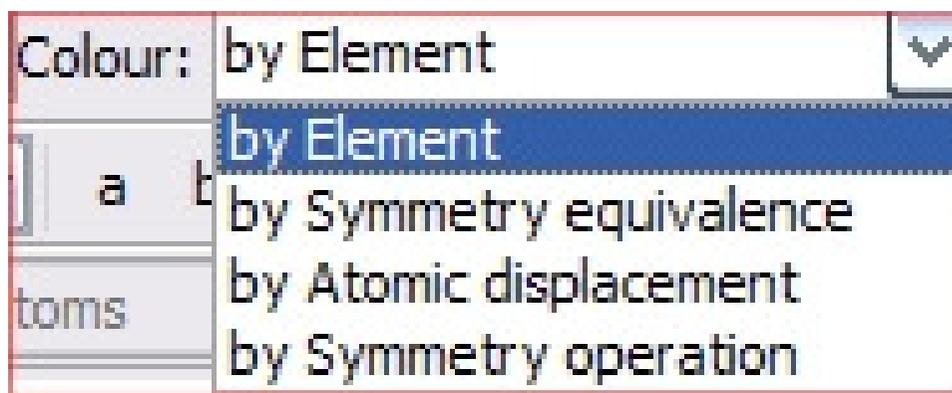
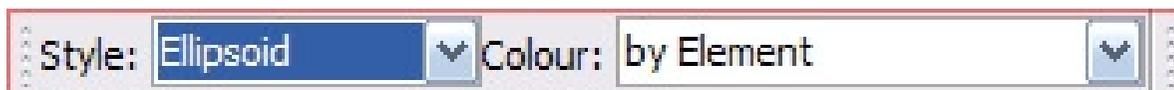
# Visualización molecular. Mercury y RasMol

- Mercury. Visualización, tipos de enlaces y átomos



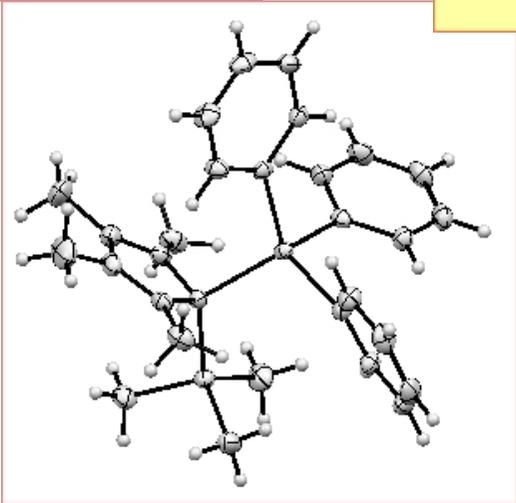
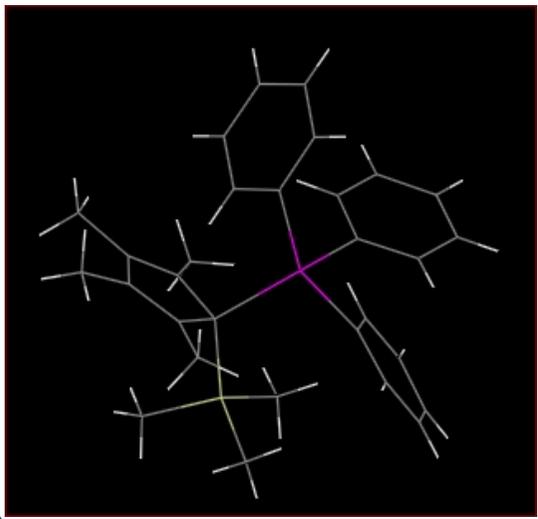
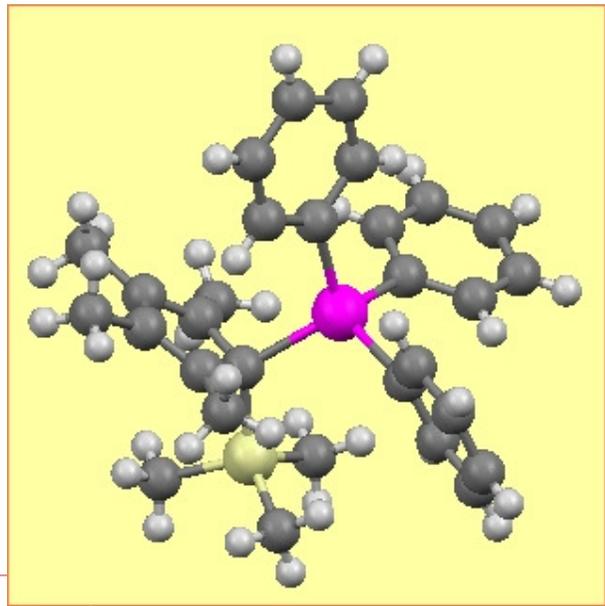
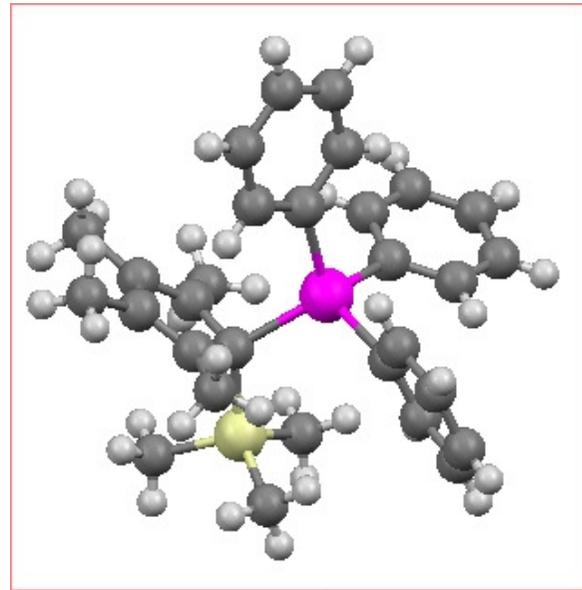
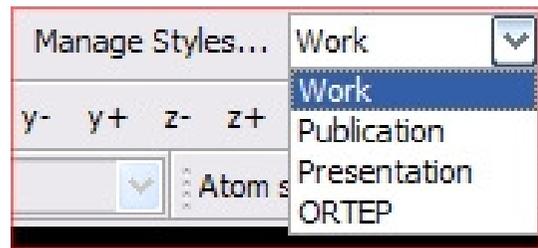
# Visualización molecular. Mercury y RasMol

- Mercury. Color de la estructura



# Visualización molecular. Mercury y RasMol

- Mercury. Estilos de vista



# Visualización molecular. Mercury y RasMol

- Mercury. Otras opciones

Default view: **b** a b c a\* b\* c\* x- x+ y- y+ z- z+ x -90 x +90 y -90 y +90 z -90 z +90 ← → ↓ ↑ zoom - zoom +

Options

<input checked="" type="checkbox"/> Show hydrogens	<input type="checkbox"/> Depth cue
<input type="checkbox"/> Show cell axes	<input type="checkbox"/> Z-Clipping
<input type="checkbox"/> Label atoms	<input type="checkbox"/> Stereo

Display Options

Display

<input type="checkbox"/> Packing	<input type="checkbox"/> Short Contact < (sum of vdW radii)	<input type="button" value="Contacts..."/>
<input type="checkbox"/> Auto centre	<input type="checkbox"/> H-Bond Default definition	<input type="button" value="More Info ▾"/>

# Visualización molecular. Mercury y RasMol

- Mercury. Etiquetado de átomos

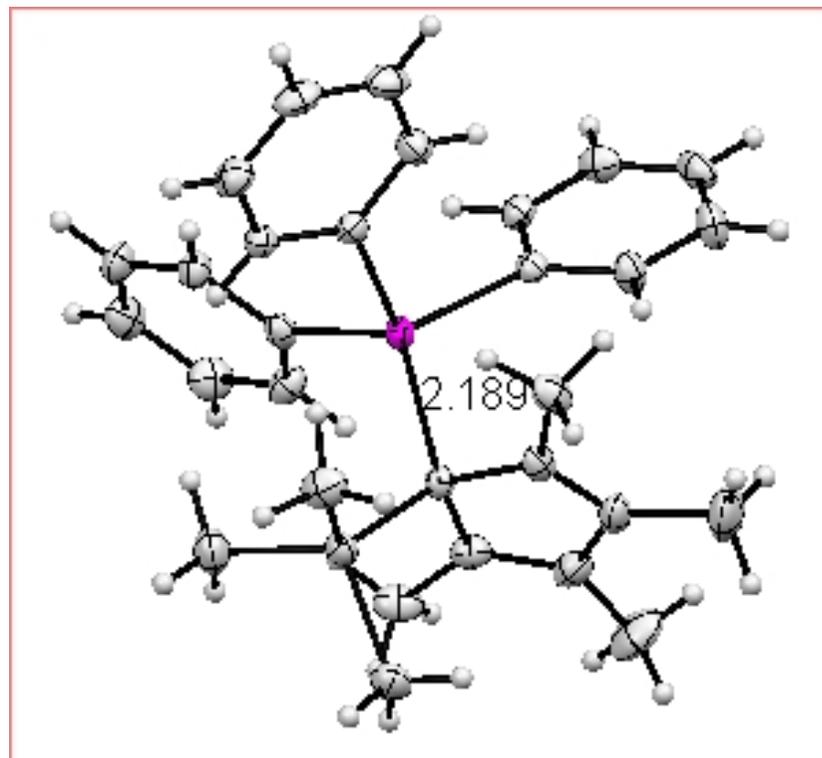
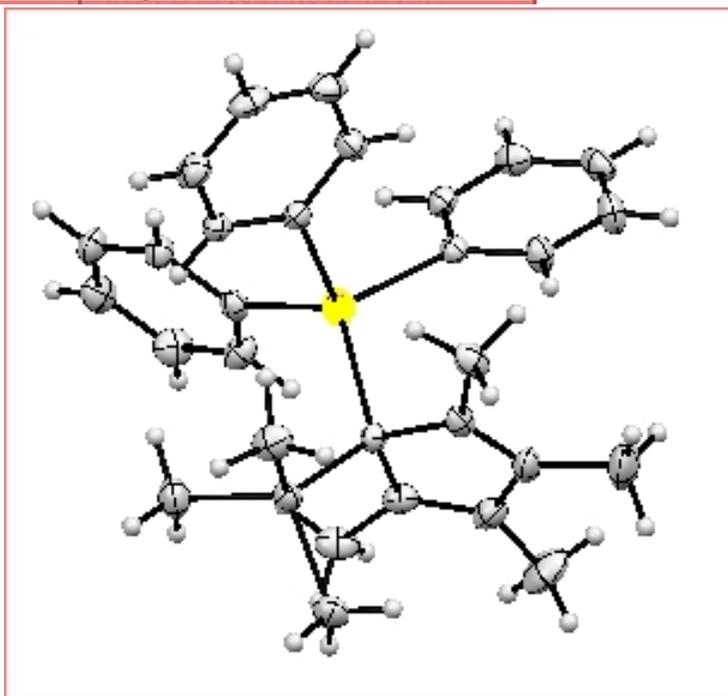
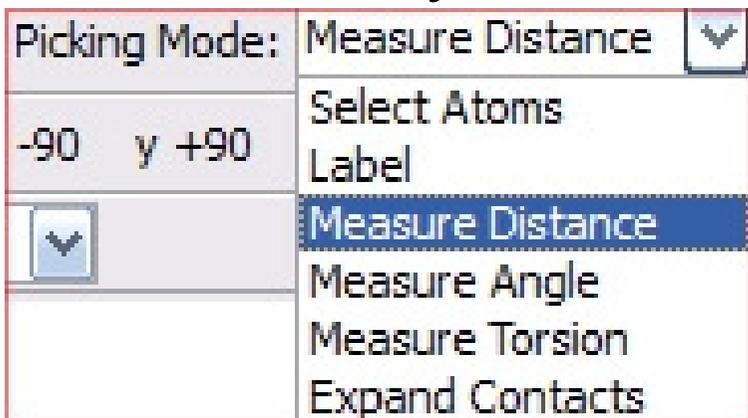
Show Labels for **Non-metal atoms** with Atom Label Atom selections:

- Non-metal atoms
- All atoms
- Carbon atoms
- Hydrogen atoms
- Non-hydrogen atoms
- Non C,H
- Metal atoms
- Non-metal atoms**
- Contact atoms
- Stereocentres

- with Uequiv
- Atom Label
  - Element
  - Atomic Number
  - Formal Charge
  - Sybyl Type
  - Stereochemistry
  - Position: Fractional
  - Position: Orthogonal
  - Occupancy
  - ADP type
  - Uequiv

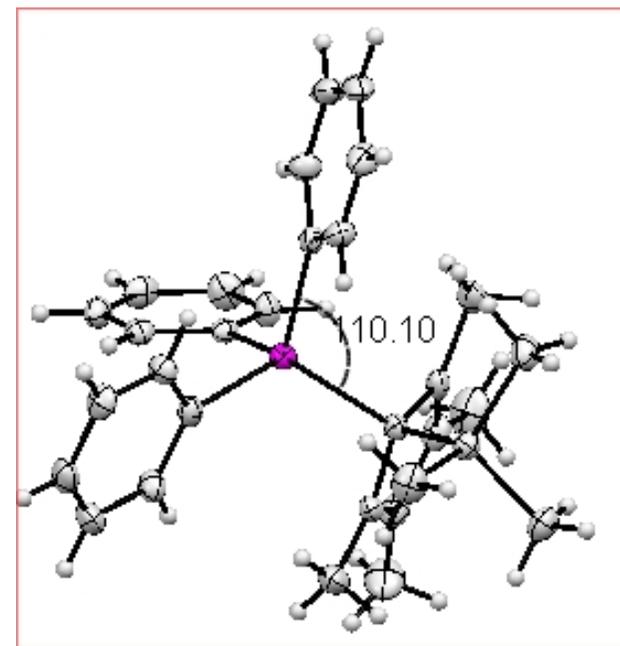
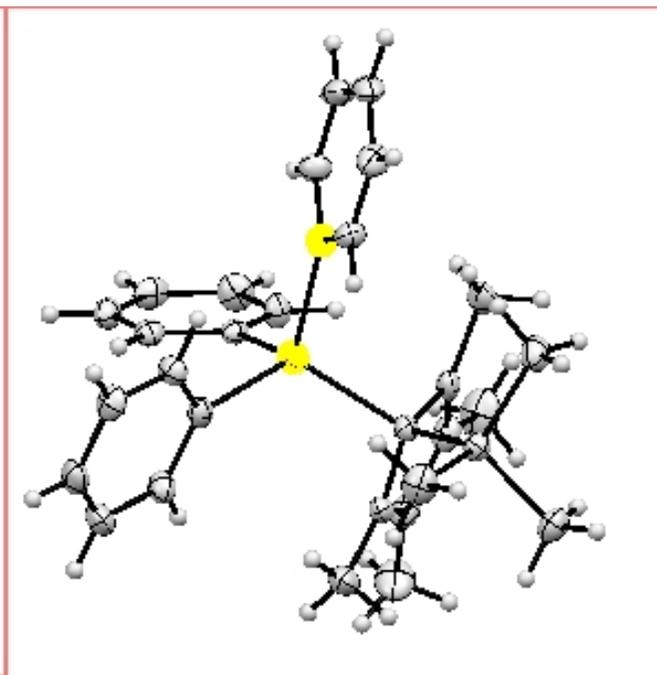
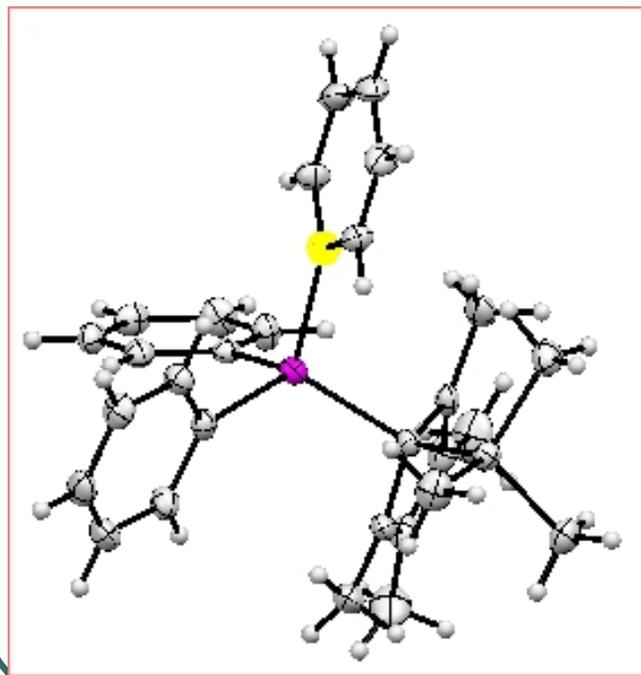
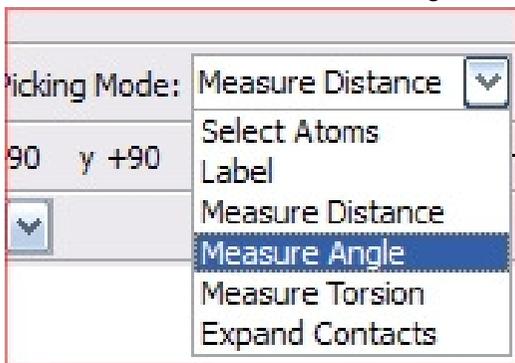
# Visualización molecular. Mercury y RasMol

- Mercury. Cálculo de distancias y ángulos de enlace



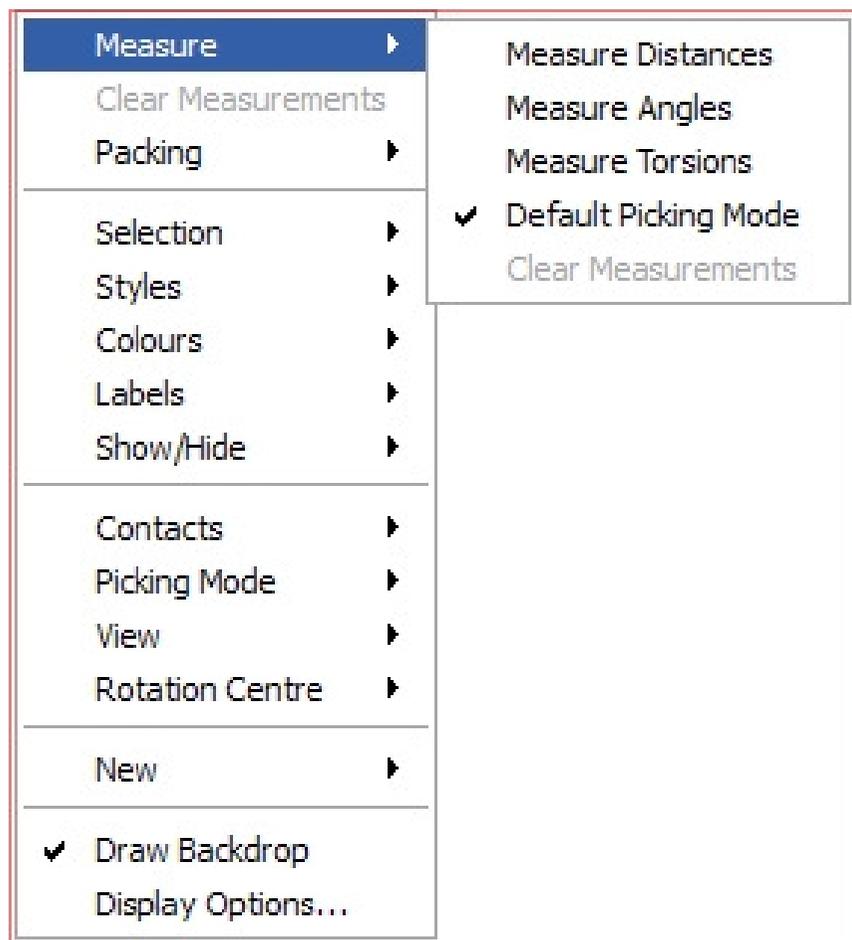
# Visualización molecular. Mercury y RasMol

- Mercury. Cálculo de distancias y ángulos de enlace

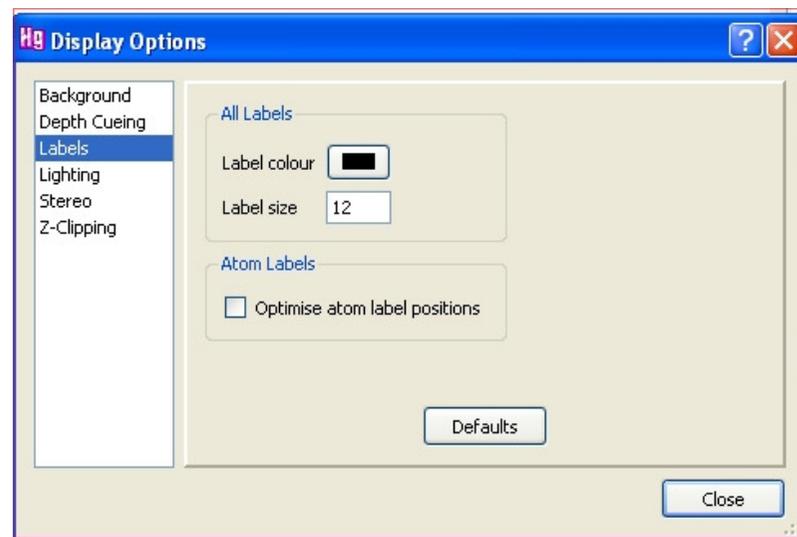
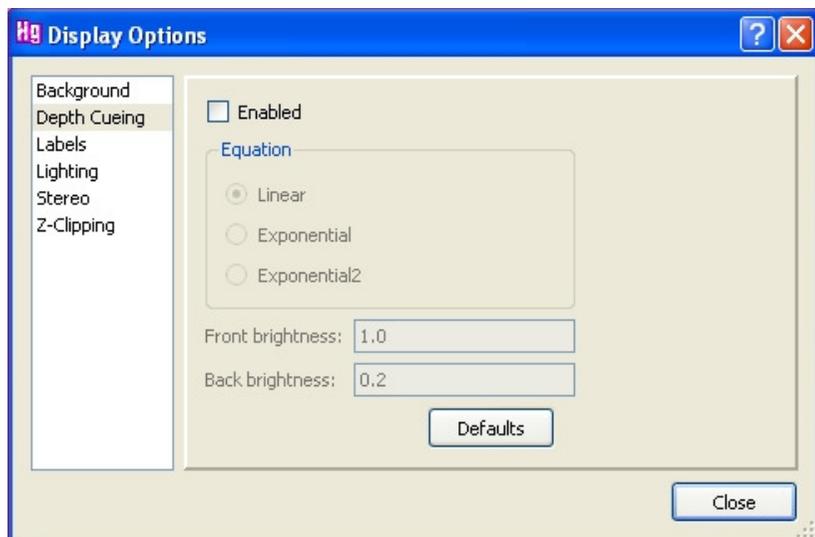
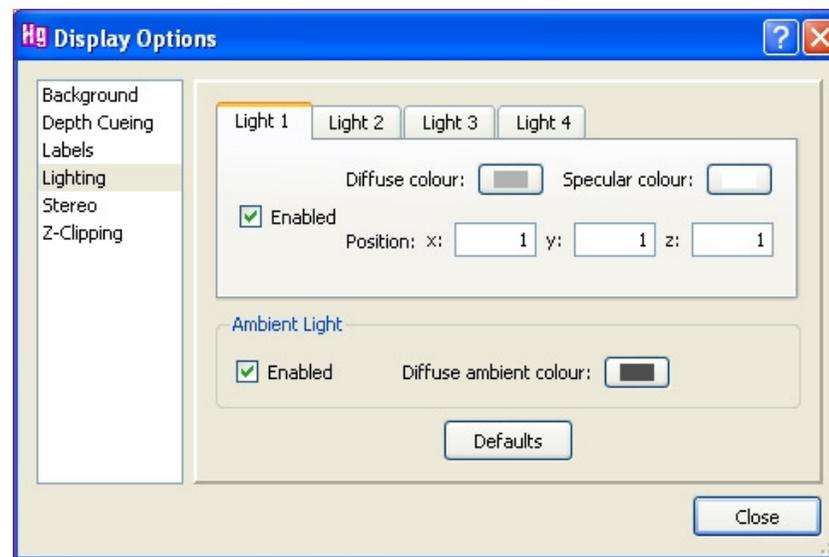
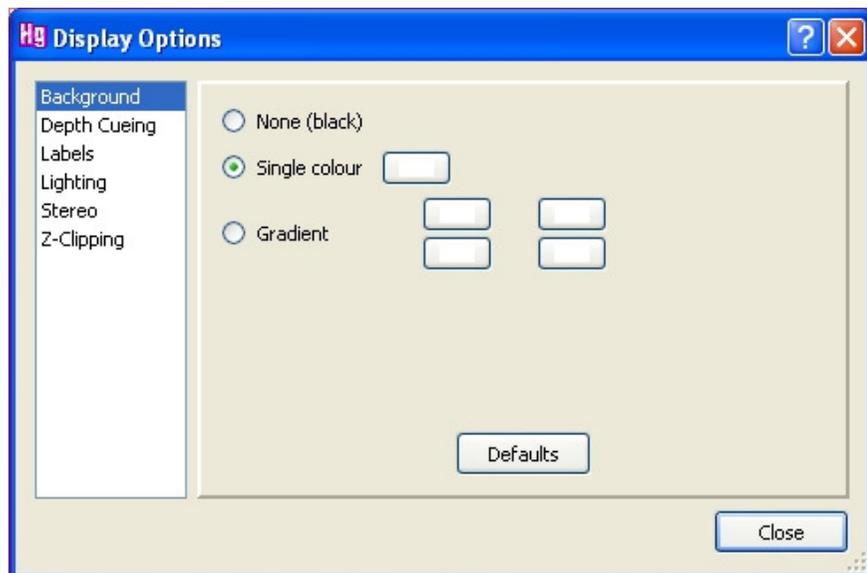


# Visualización molecular. Mercury y RasMol

- Mercury. Otras configuraciones

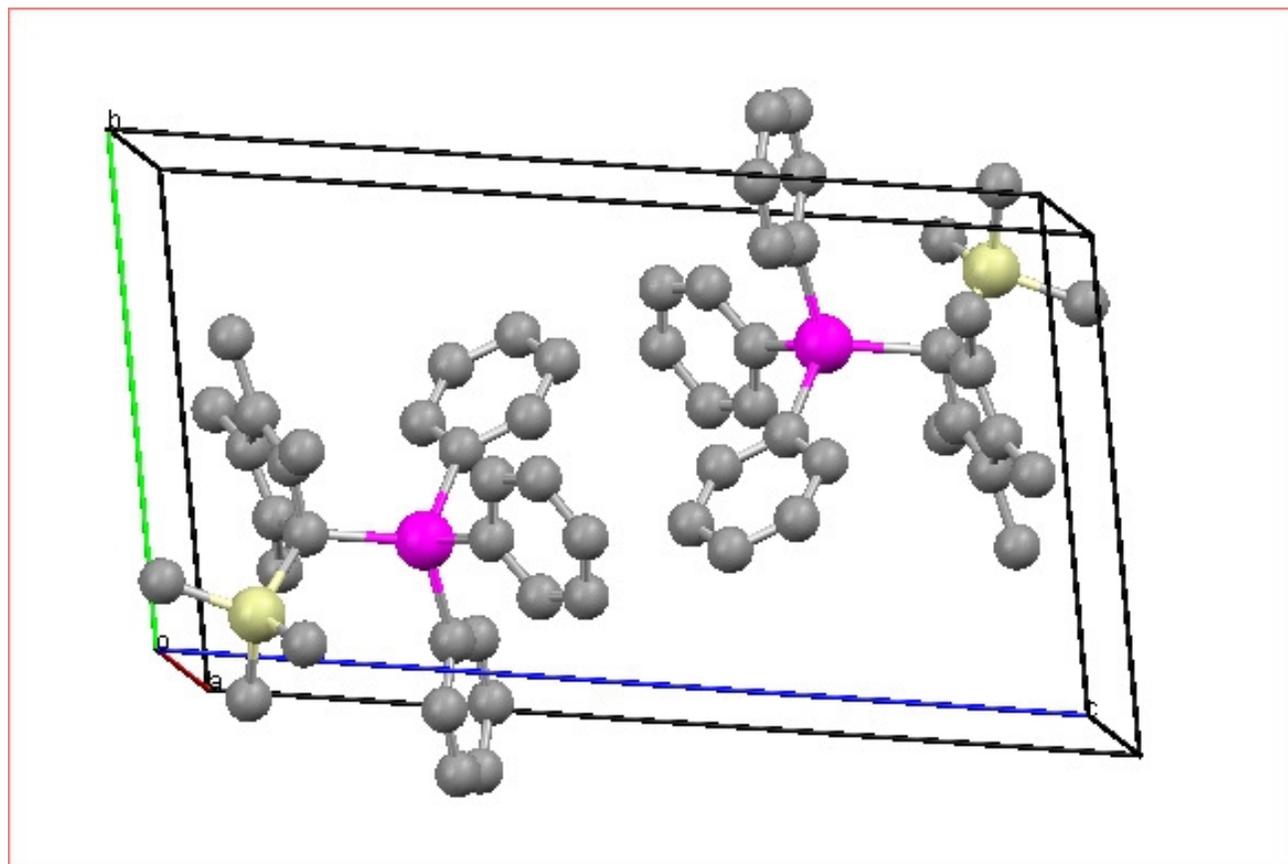


# Visualización molecular. Mercury y RasMol

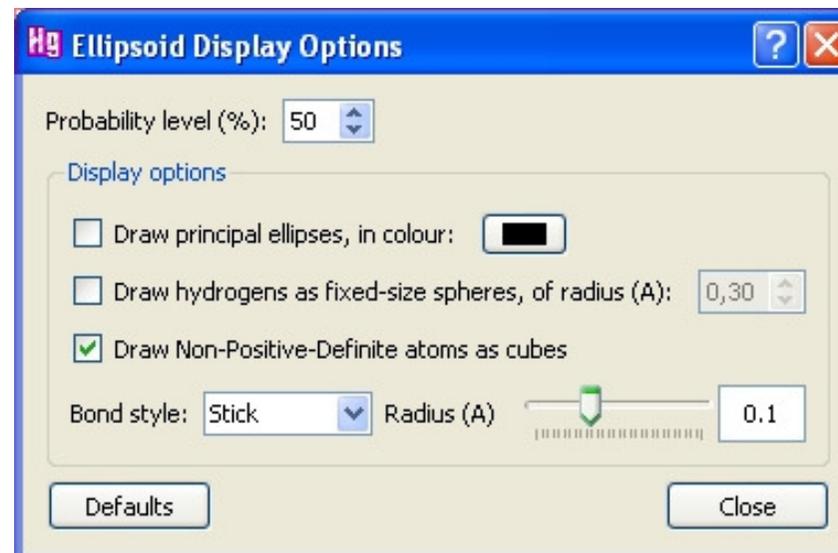
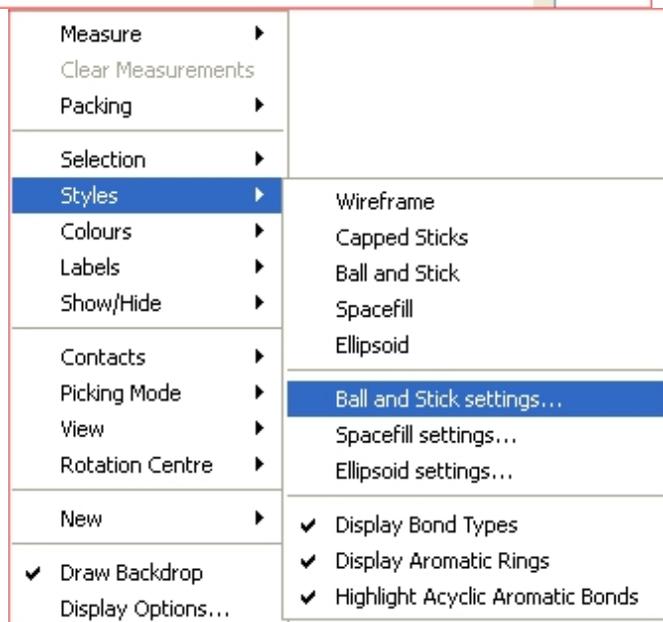
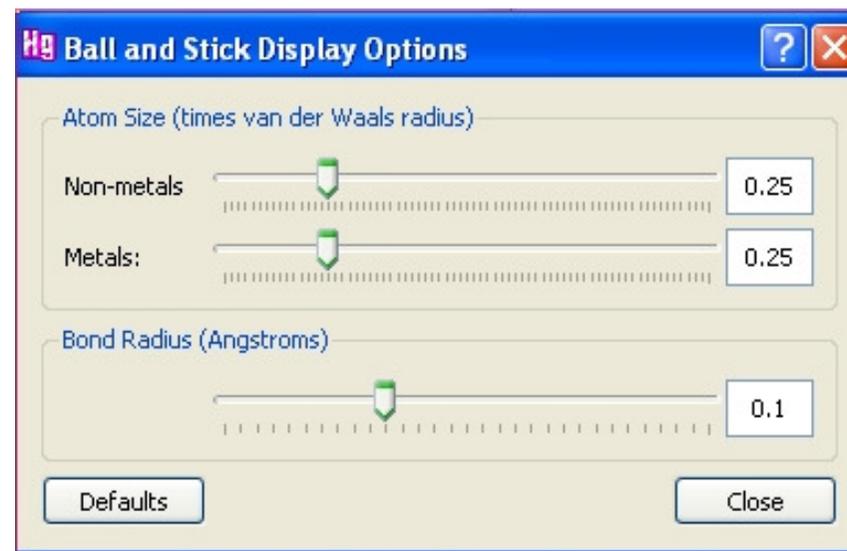
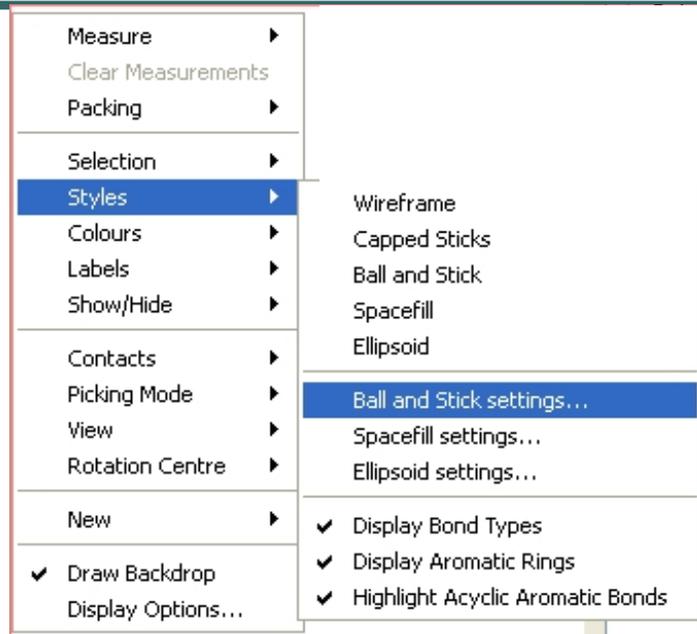


# Visualización molecular. Mercury y RasMol

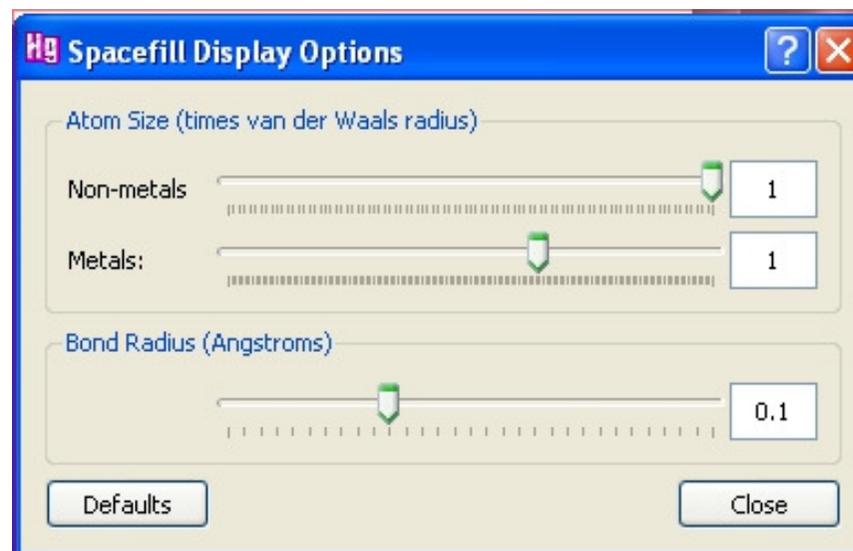
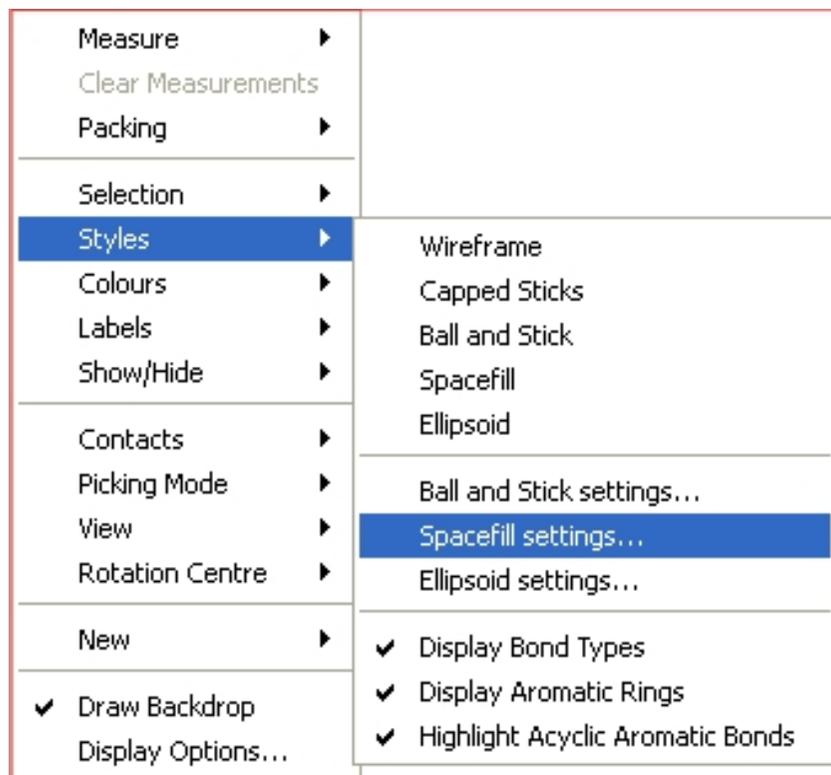
Measure	▶	
Clear Measurements		
Packing	▶	Molecule
		Packing
Selection	▶	
Styles	▶	
Colours	▶	
Labels	▶	
Show/Hide	▶	
<hr/>		
Contacts	▶	
Picking Mode	▶	
View	▶	
Rotation Centre	▶	
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New	▶	
<hr/>		
✓ Draw Backdrop		
Display Options...		



# Visualización molecular. Mercury y RasMol

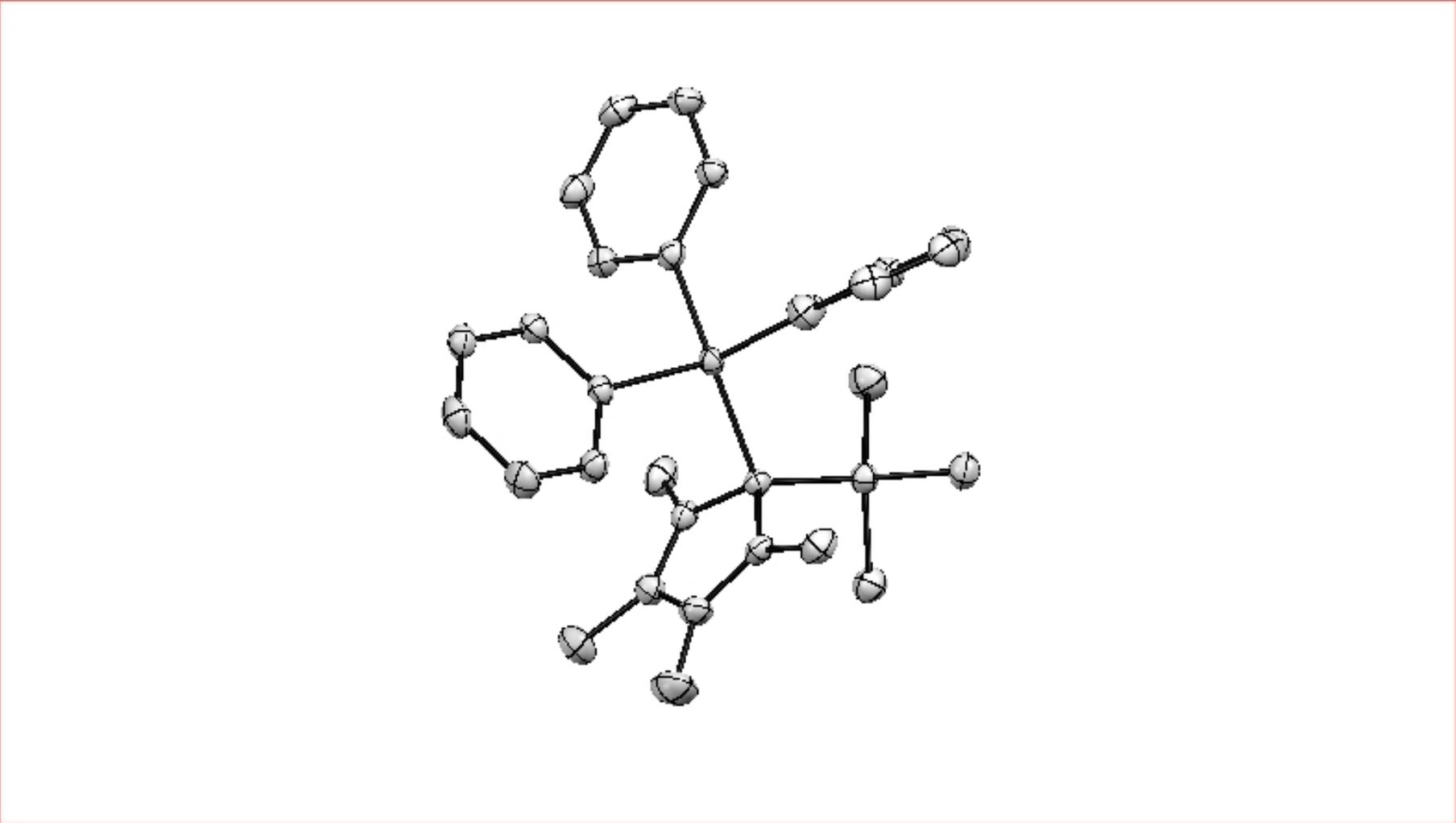


# Visualización molecular. Mercury y RasMol

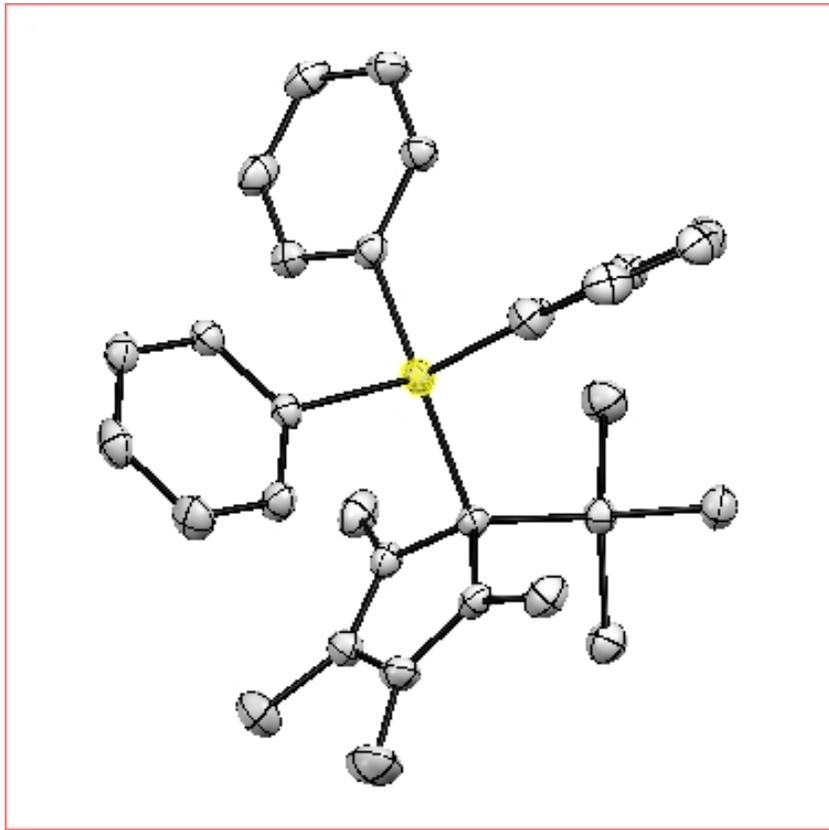


# Visualización molecular. Mercury y RasMol

Style: Ellipsoid    Colour: by Element    Manage Styles...    ORTEP

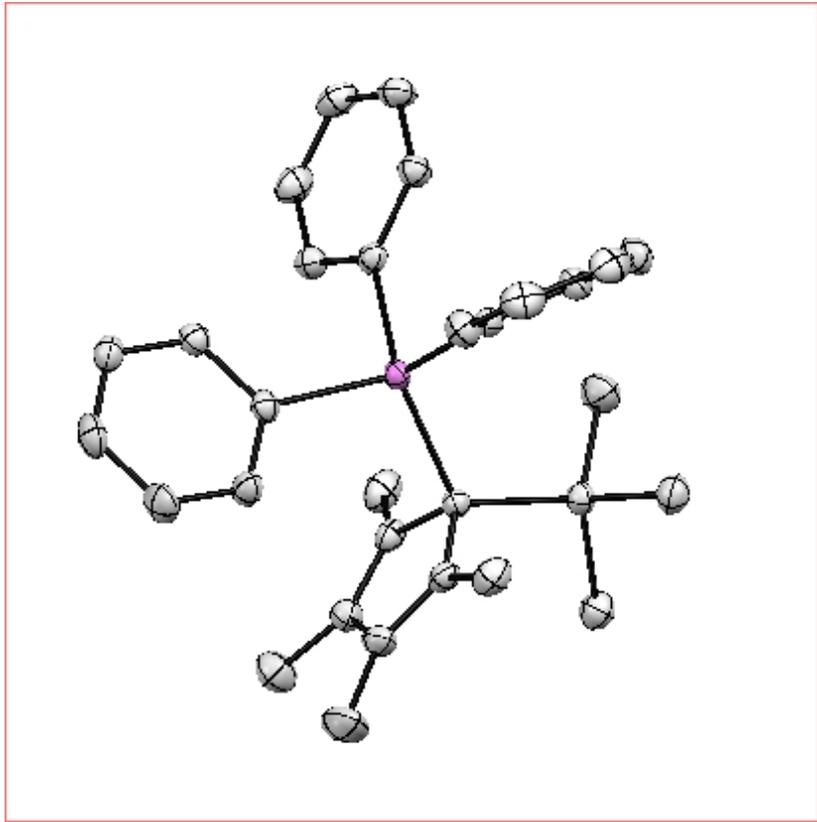


# Visualización molecular. Mercury y RasMol



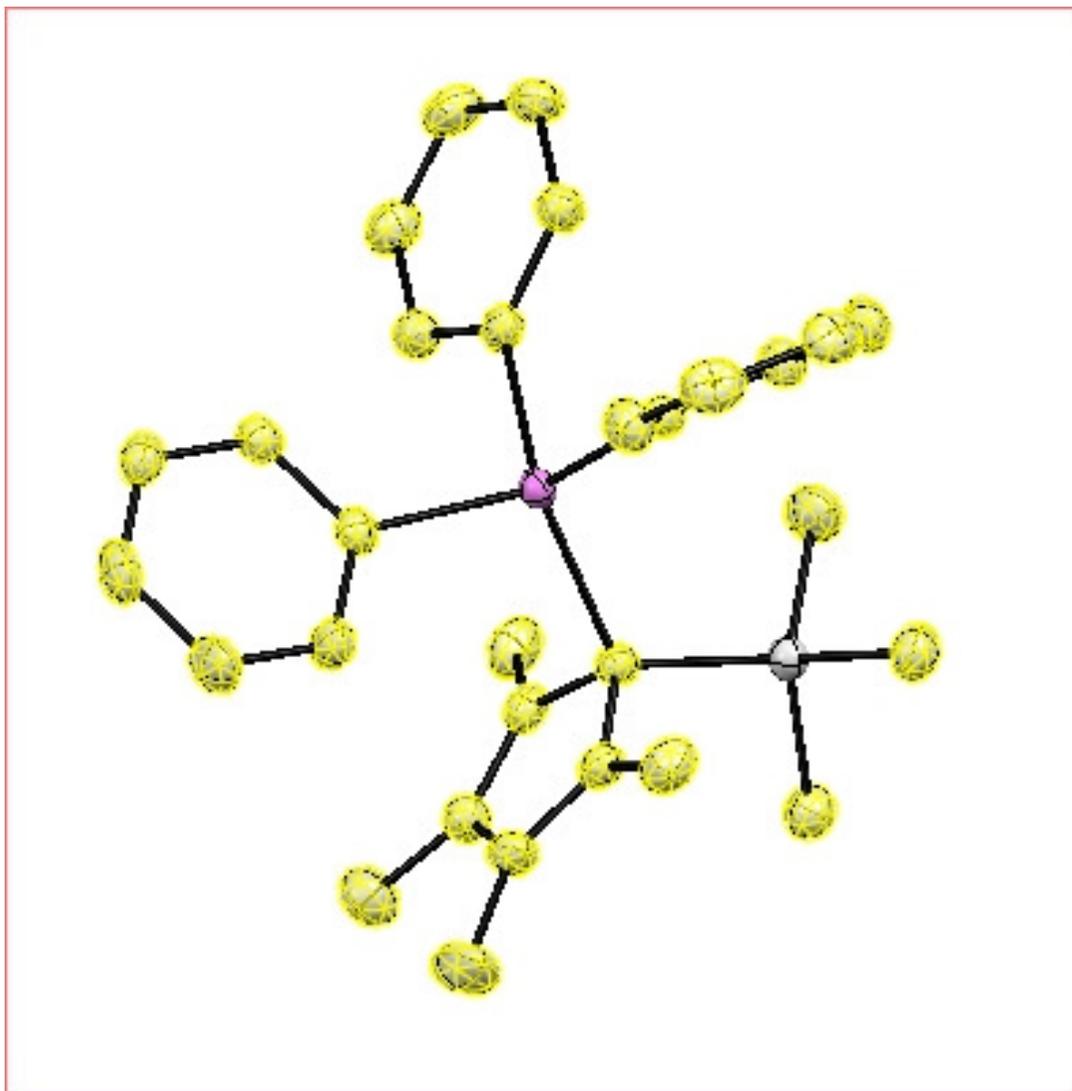
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Clear Measurements	Colour By Element
Packing ▶	Colour By Symmetry Equivalence
Selection ▶	Colour By Atomic Displacement
Styles ▶	Colour By Symmetry Operation
<b>Colours ▶</b>	Element colours...
Labels ▶	Symmetry Equivalence colours...
Show/Hide ▶	
Contacts ▶	White
Picking Mode ▶	Light Grey
View ▶	Grey
Rotation Centre ▶	Dark Grey
New ▶	Black
✓ Draw Backdrop	Pink
Display Options...	Red
	Orange
	Yellow
	Light Green
	Green
	Light Blue
	Blue
	Purple
	<b>Violet</b>
	Magenta
	Colour...

# Visualización molecular. Mercury y RasMol



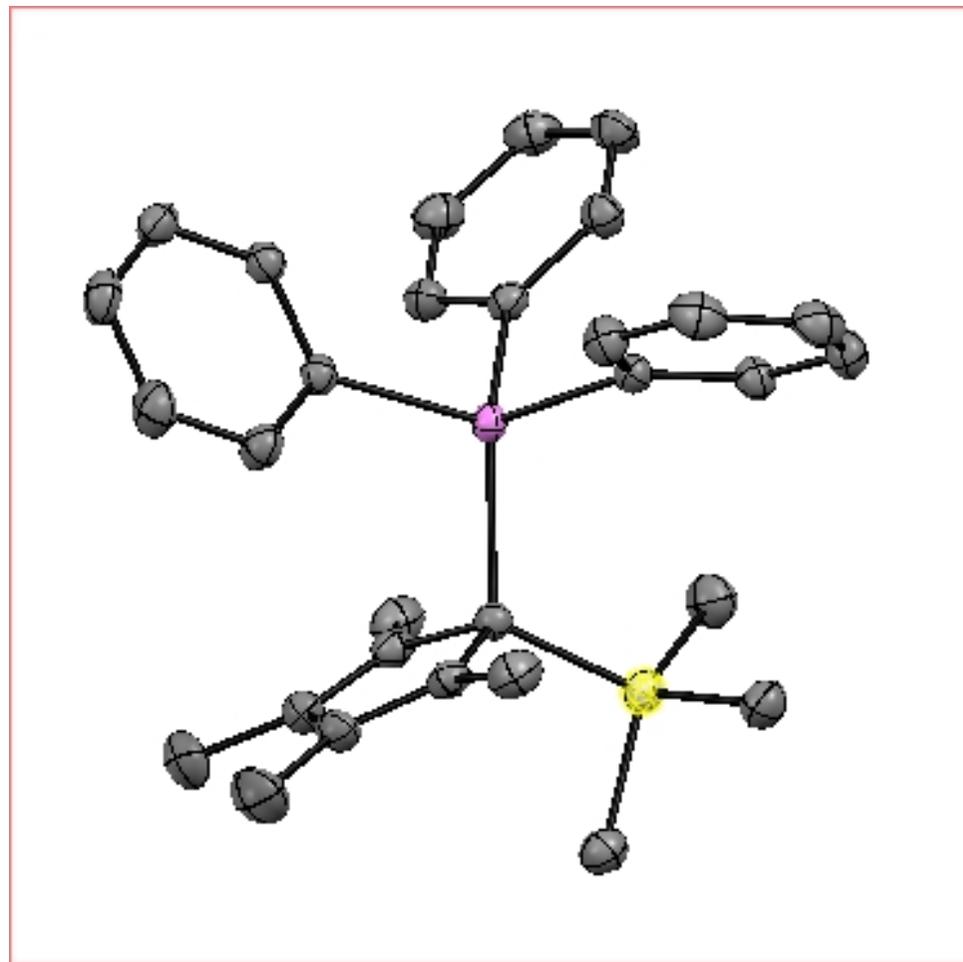
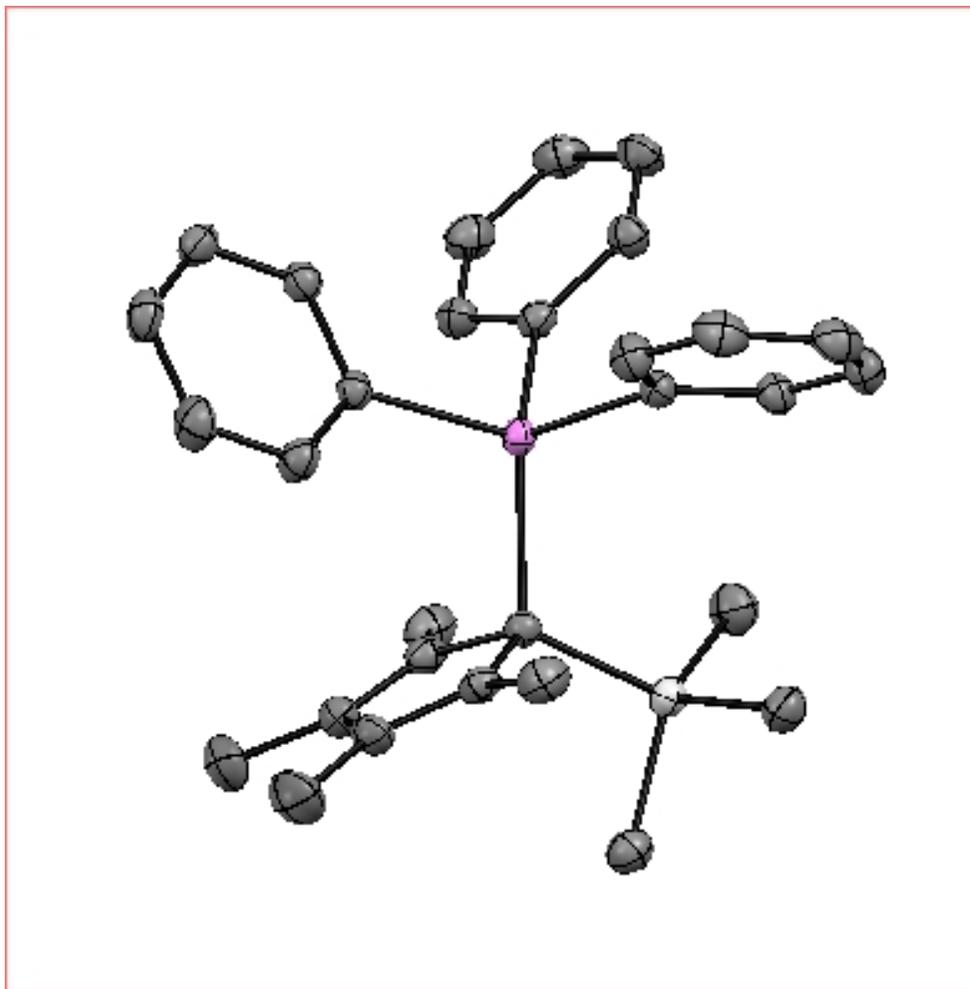
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Clear Measurements	
Packing ▶	
<b>Selection ▶</b>	Select All Ctrl+A
Styles ▶	Select Molecules...
Colours ▶	Select Atoms...
Labels ▶	<b>Select ▶</b>
Show/Hide ▶	Select Hydrogen
	Select Non-Hydrogen
	<b>Select Carbons</b>
	Select Non-H, C
	Select Metal Atoms
	Select Non-Metal Atoms
Contacts ▶	Select Contact Atoms
Picking Mode ▶	Select Stereocentres
View ▶	Deselect Metal Atoms
Rotation Centre ▶	Deselect Non-Metal Atoms
	Deselect Stereocentres
New ▶	
✓ Draw Backdrop	
Display Options...	

# Visualización molecular. Mer



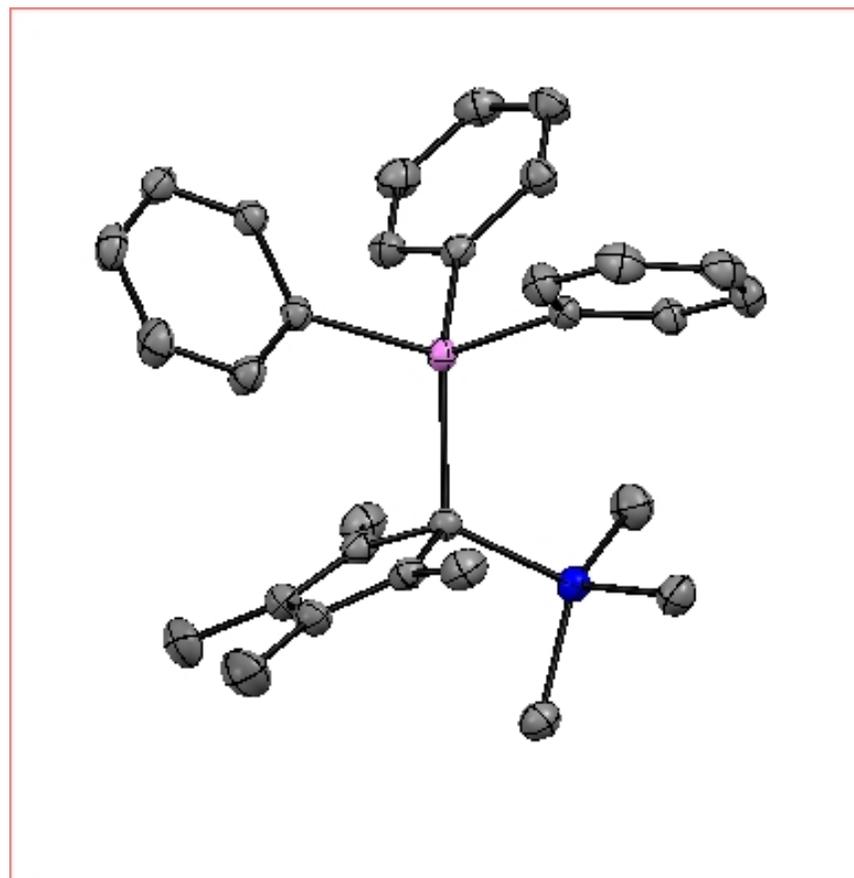
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Styles ▶	
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Labels ▶	Colour By Element
Show/Hide ▶	Colour By Symmetry Equivalence
	Colour By Atomic Displacement
	Colour By Symmetry Operation
Contacts ▶	
Picking Mode ▶	Element colours...
View ▶	Symmetry Equivalence colours...
Rotation Centre ▶	
New ▶	White
✓ Draw Backdrop	Light Grey
Display Options...	<b>Grey</b>
	Dark Grey
	Black
	Pink
	Red
	Orange
	Yellow
	Light Green
	Green
	Light Blue
	Blue
	Purple
	Violet
	Magenta
	>> Colour...

# Visualización molecular. Mercury y RasMol



# Visualización molecular. Mercury y RasMol

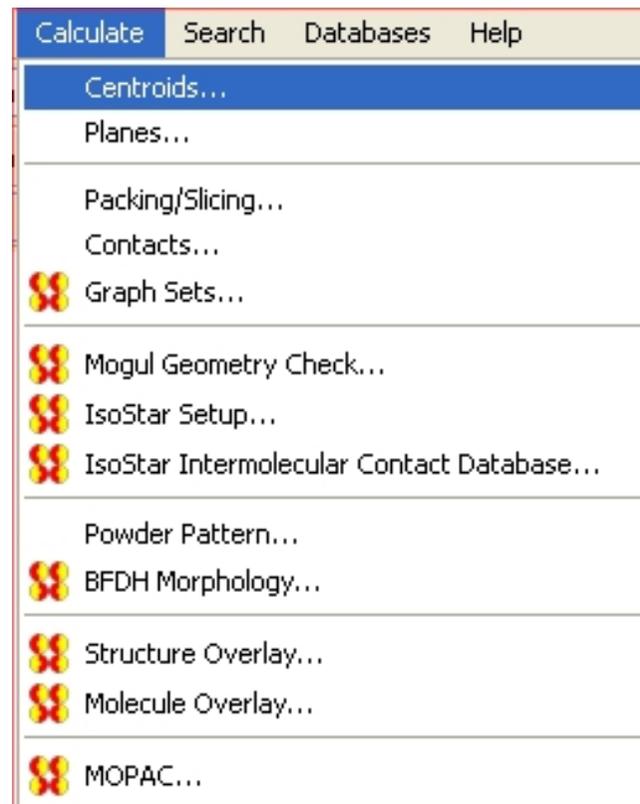
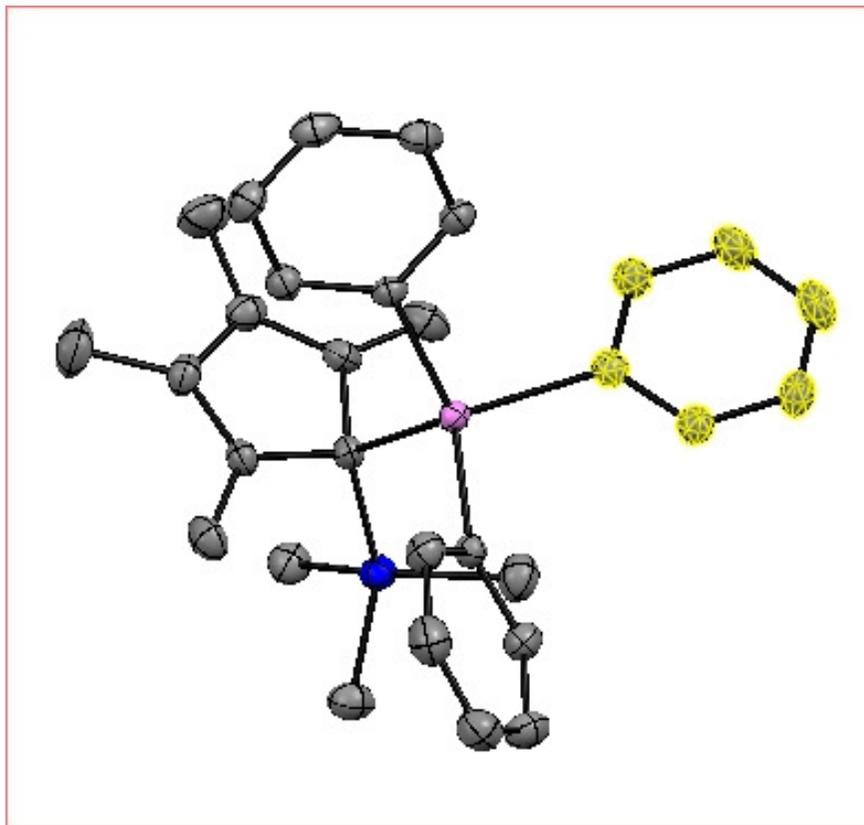
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Clear Measurements	
Packing ▶	
Selection ▶	
Styles ▶	
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Labels ▶	Colour By Element
Show/Hide ▶	Colour By Symmetry Equivalence
	Colour By Atomic Displacement
	Colour By Symmetry Operation
Contacts ▶	Element colours...
Picking Mode ▶	Symmetry Equivalence colours...
View ▶	
Rotation Centre ▶	
New ▶	White
✓ Draw Backdrop	Light Grey
Display Options...	Grey
	Dark Grey
	Black
	Pink
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	Green
	Light Blue
	<b>Blue</b>
	Purple
	Violet
	Magenta
	Colour...



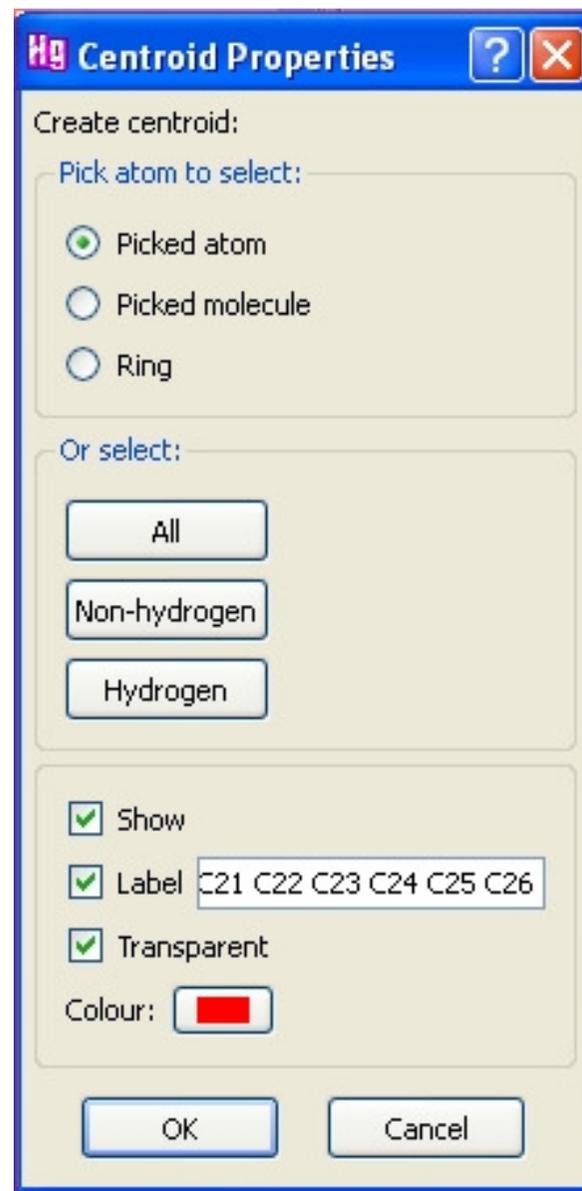
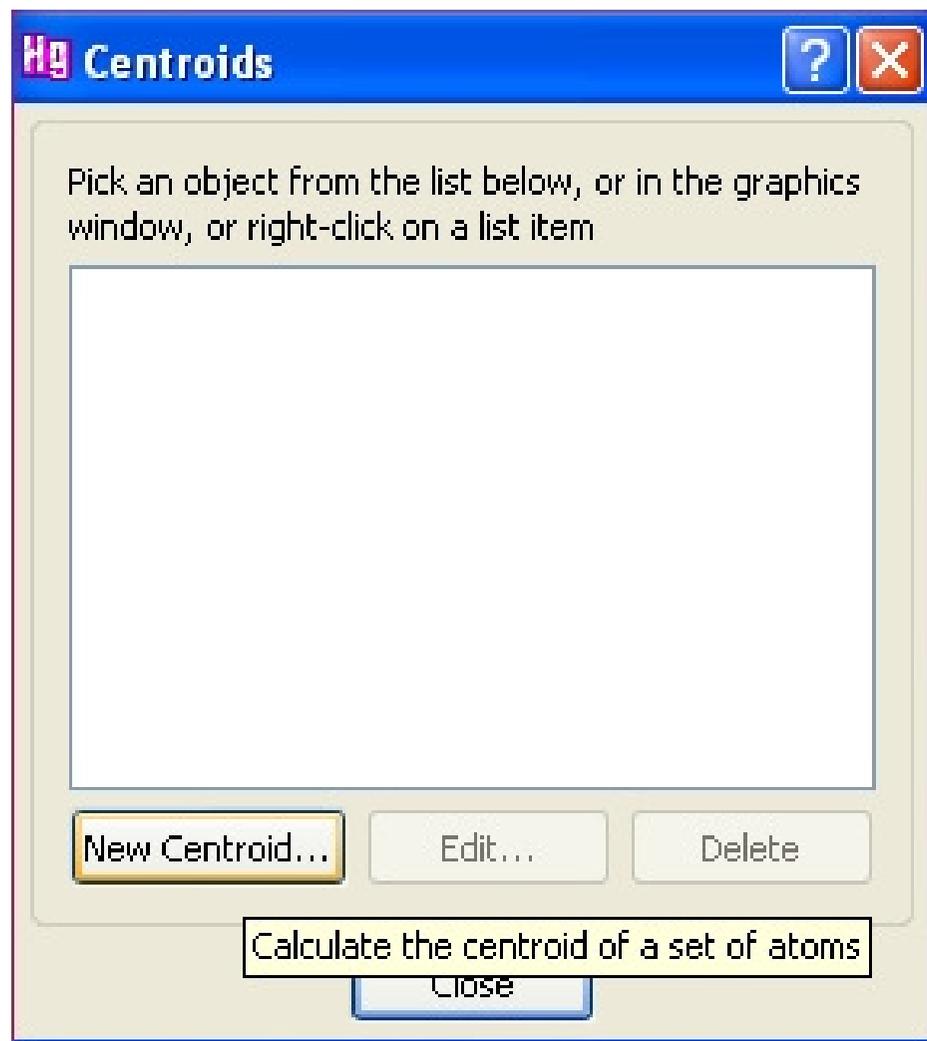
# Visualización molecular. Mercury y RasMol

Para poner etiquetas lo mismo, señalando los átomos  
o poner todas las etiquetas

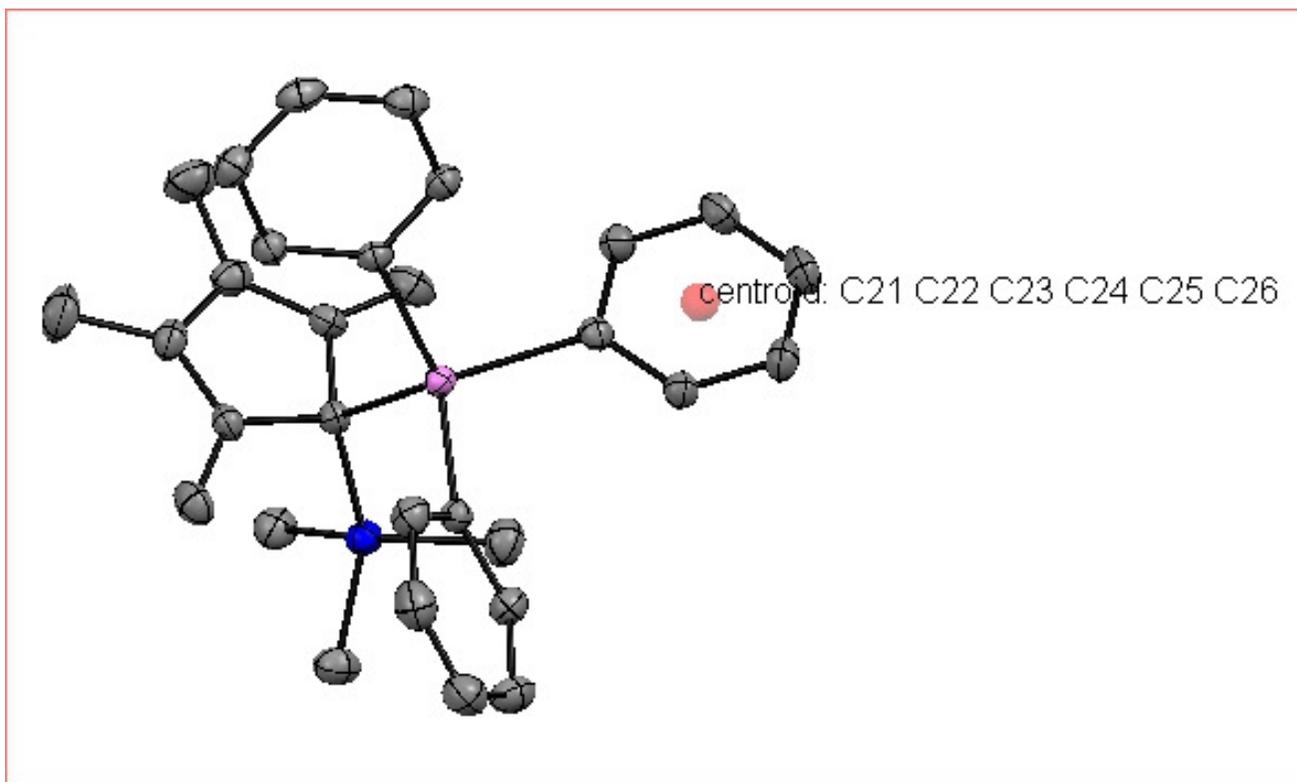
Para calcular centroides (muy útil en anillos)



# Visualización molecular. Mercury y RasMol

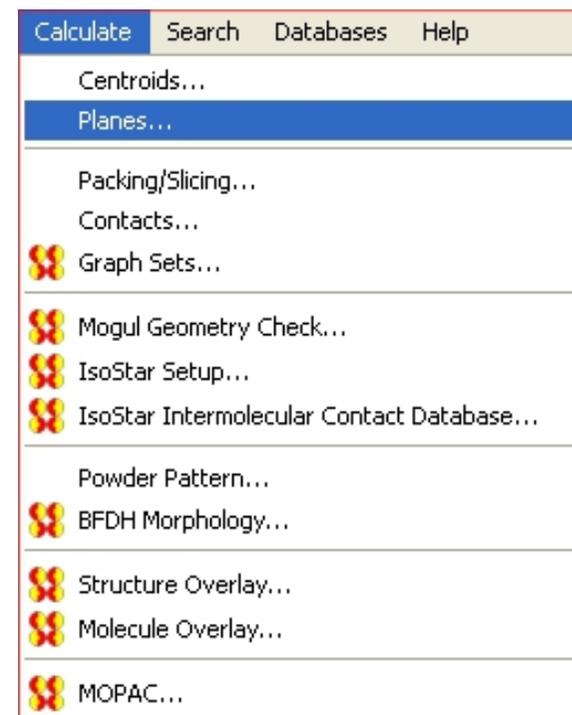
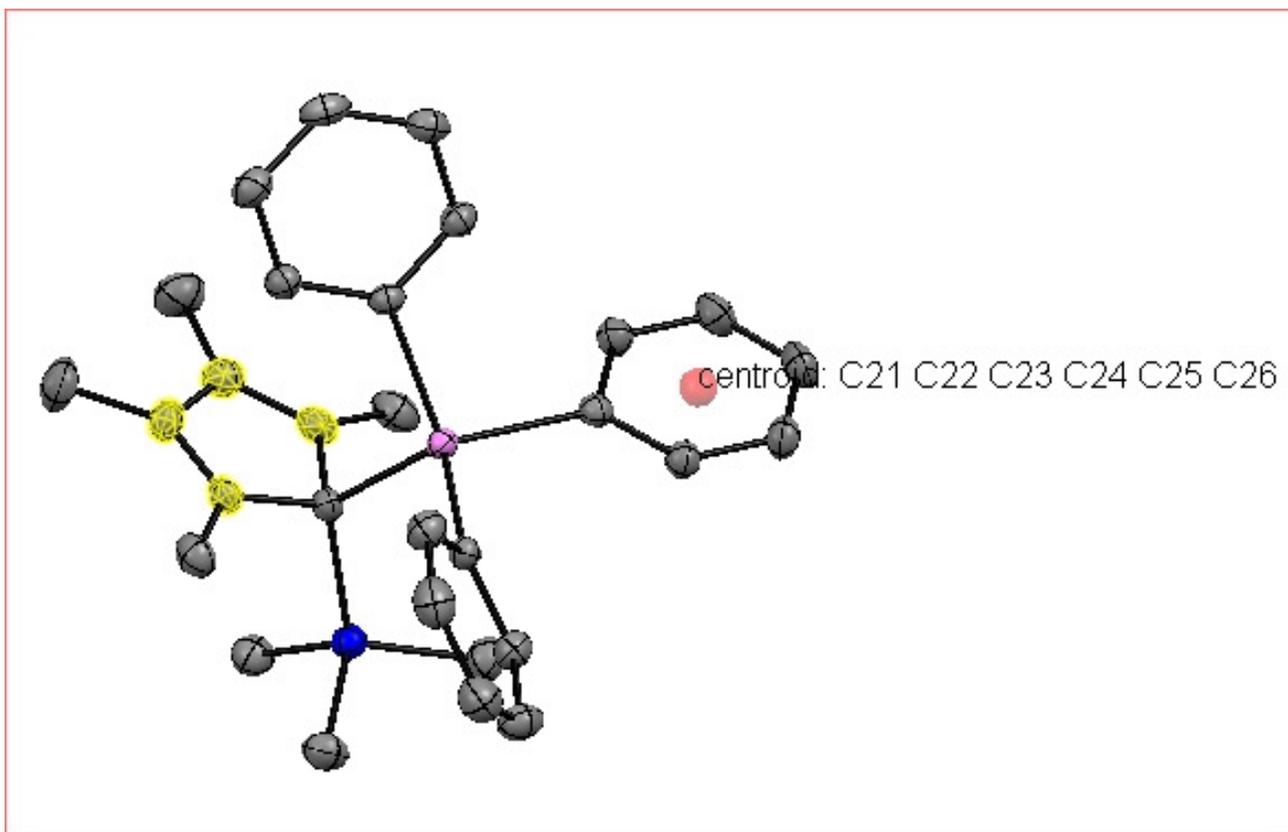


# Visualización molecular. Mercury y RasMol

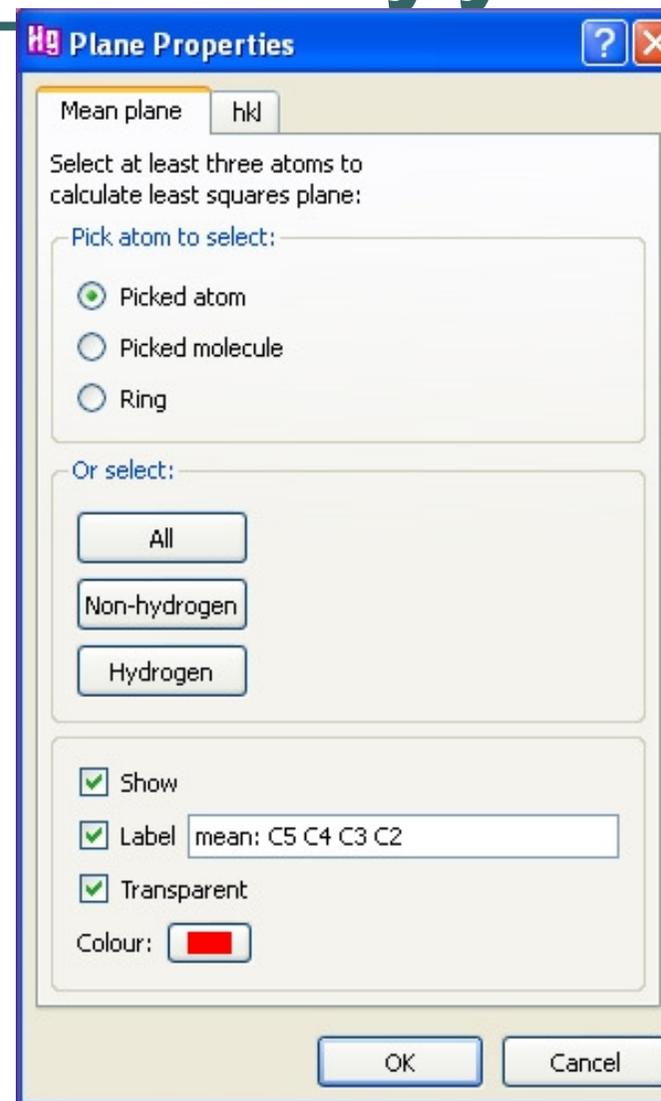
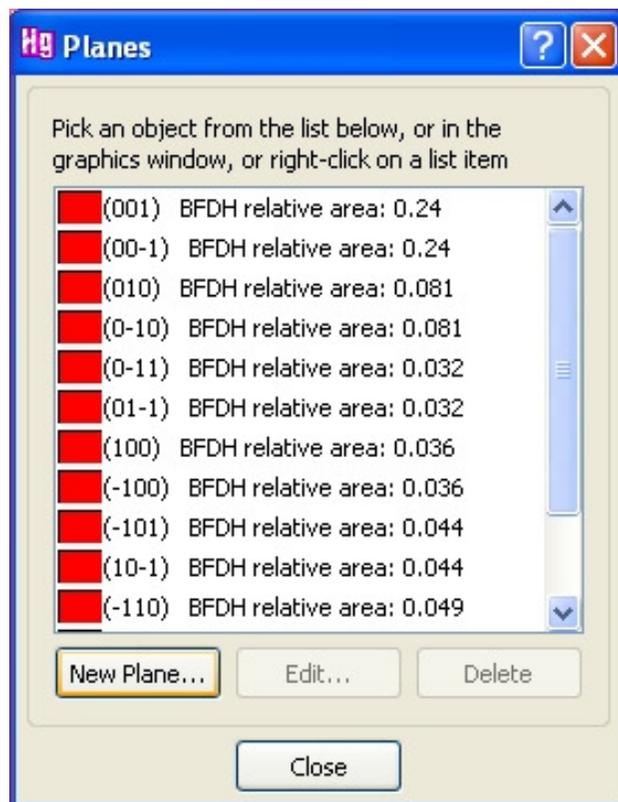


# Visualización molecular. Mercury y RasMol

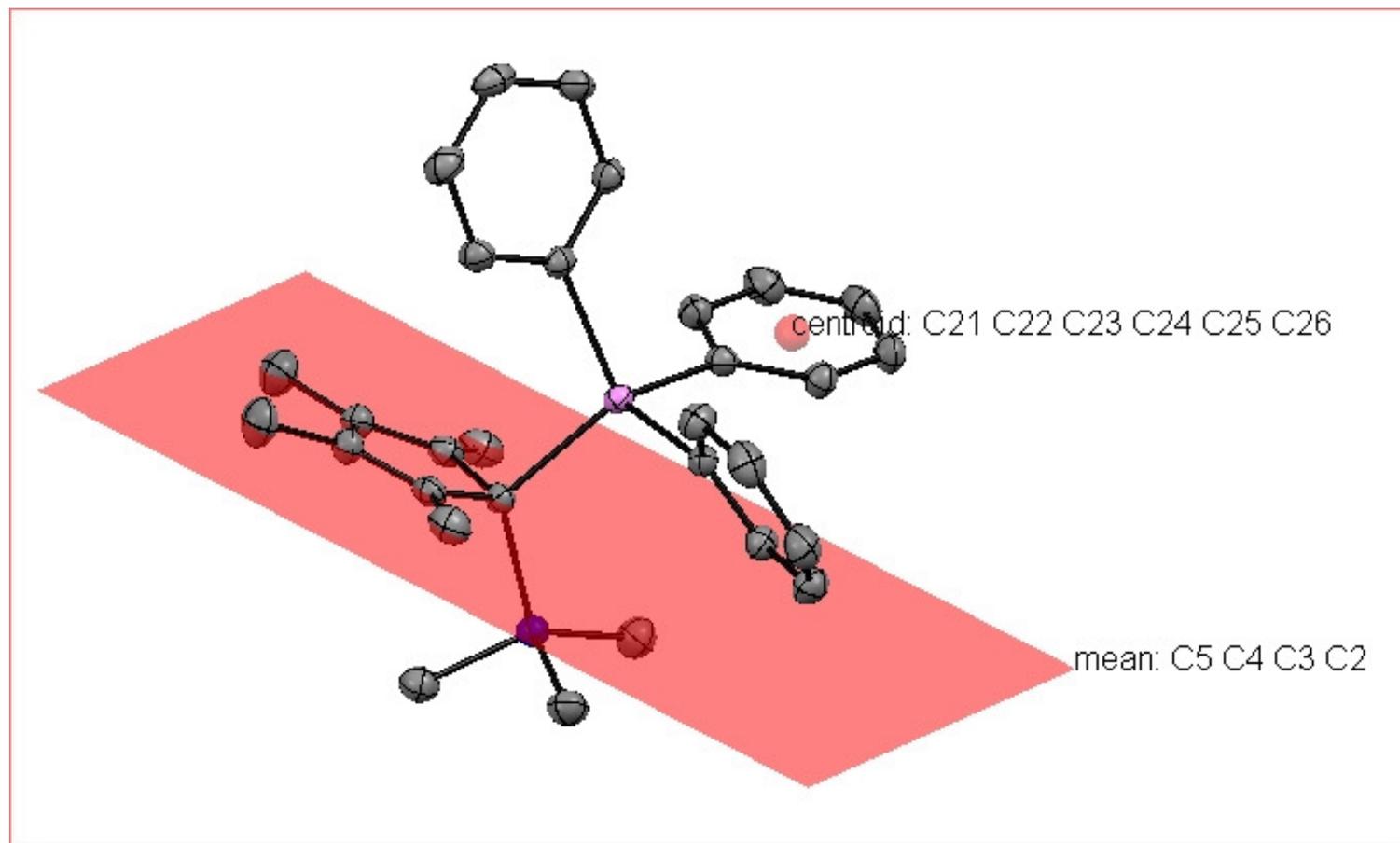
Para calcular planos (muy útil en anillos)



# Visualización molecular. Mercury y RasMol



# Visualización molecular. Mercury y RasMol



# Visualización molecular. Mercury y RasMol

Delete Object

Clear All Objects

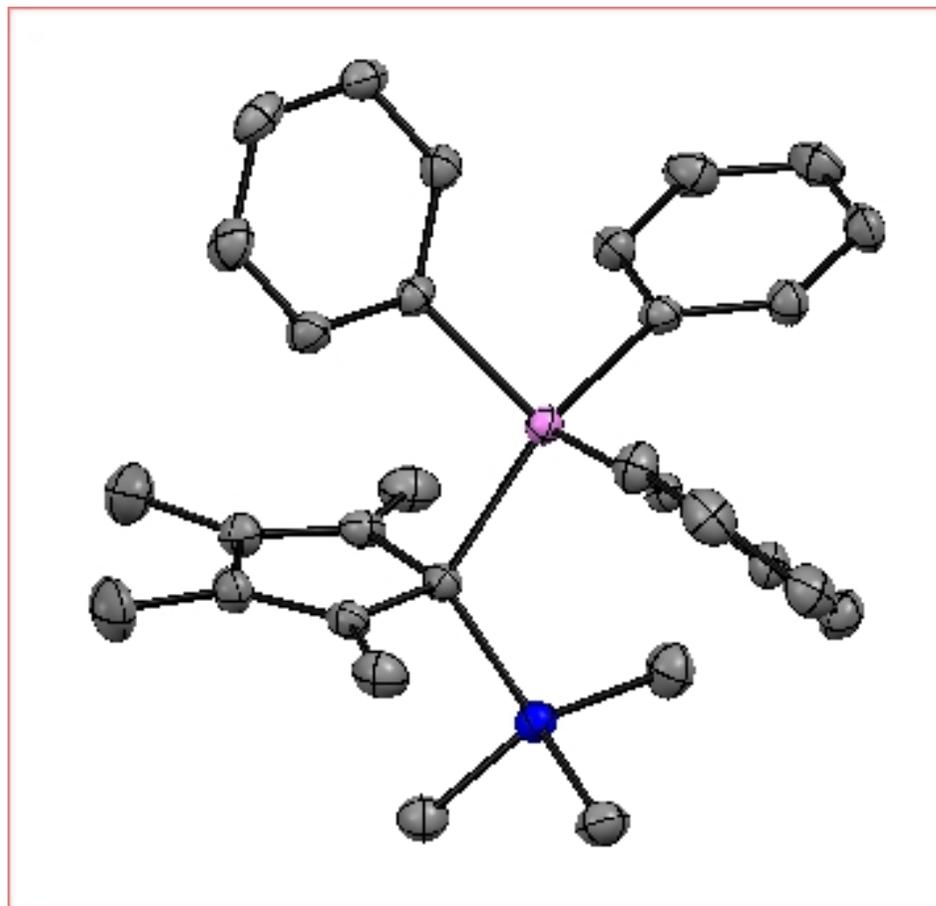
Colours ▶

Labels ▶

Show/Hide ▶

View along plane

View perpendicular to plane



# Visualización molecular. Mercury y RasMol

Display Options

Display

Packing

Auto centre

Short Contact < (sum of vdW radii)

H-Bond Default definition

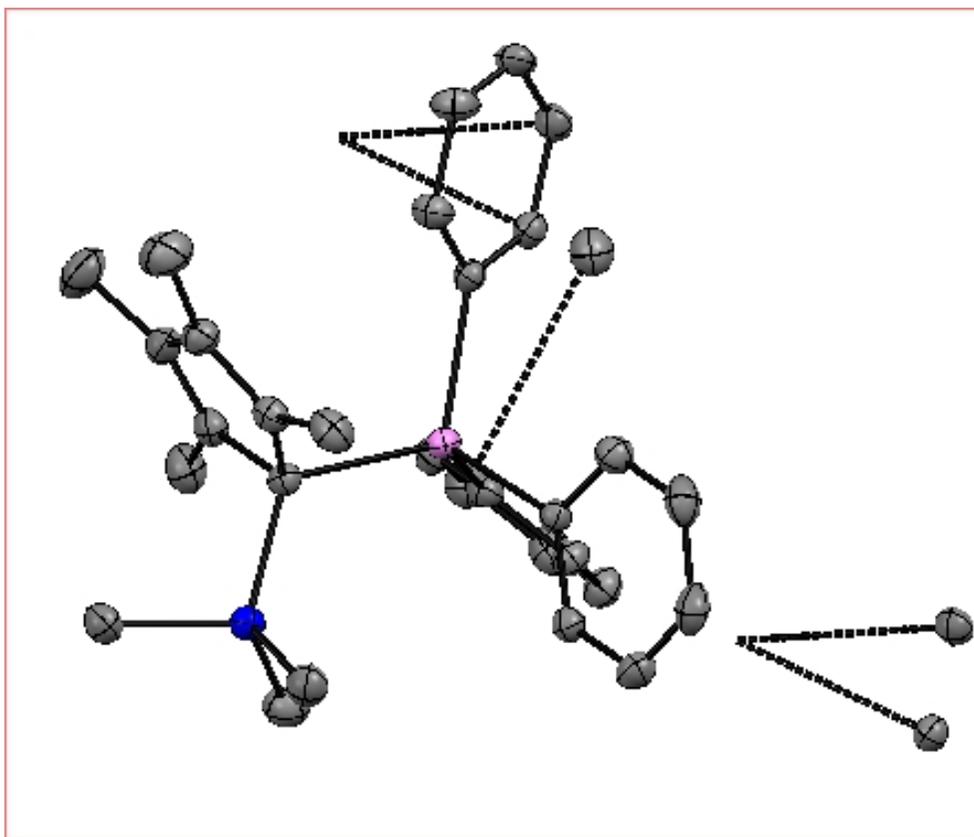
Reset

Contacts...

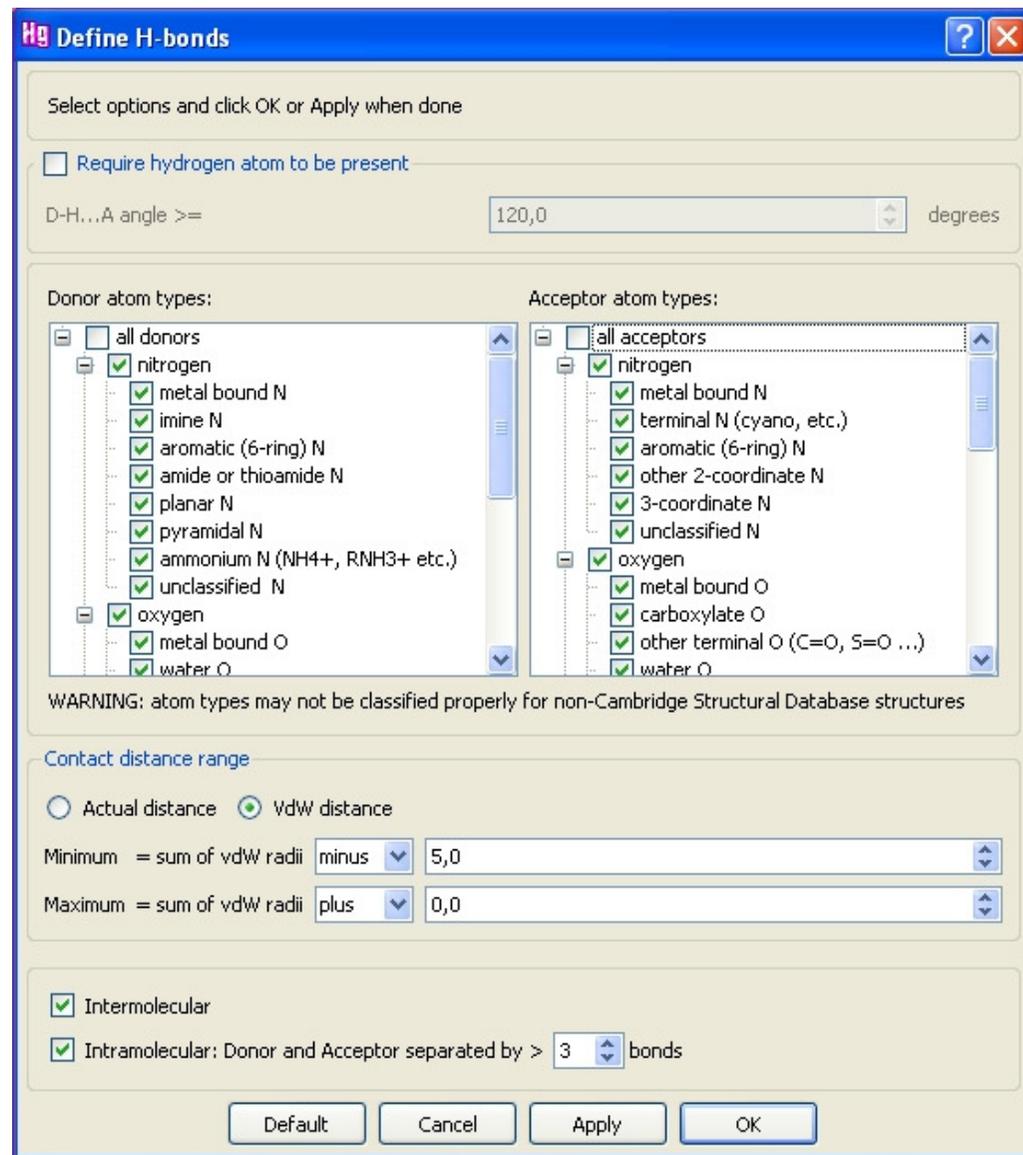
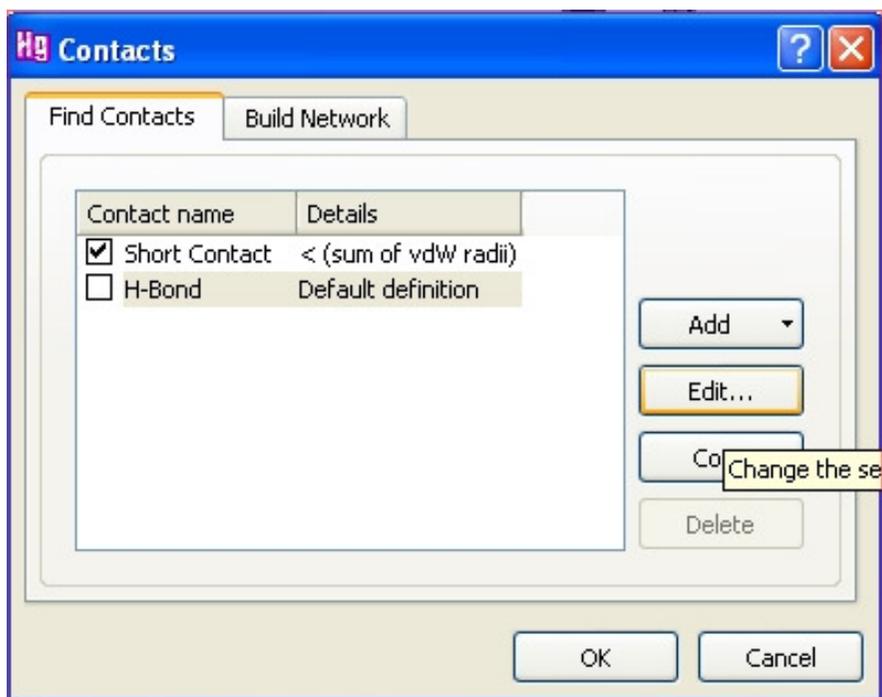
More Info ▾

Powder...

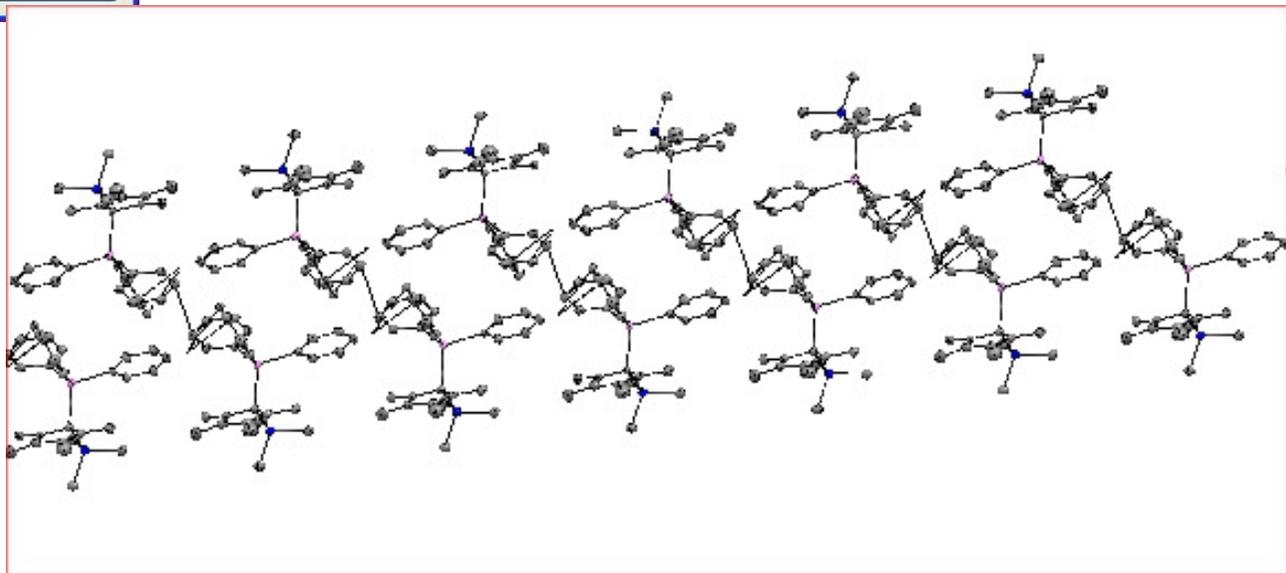
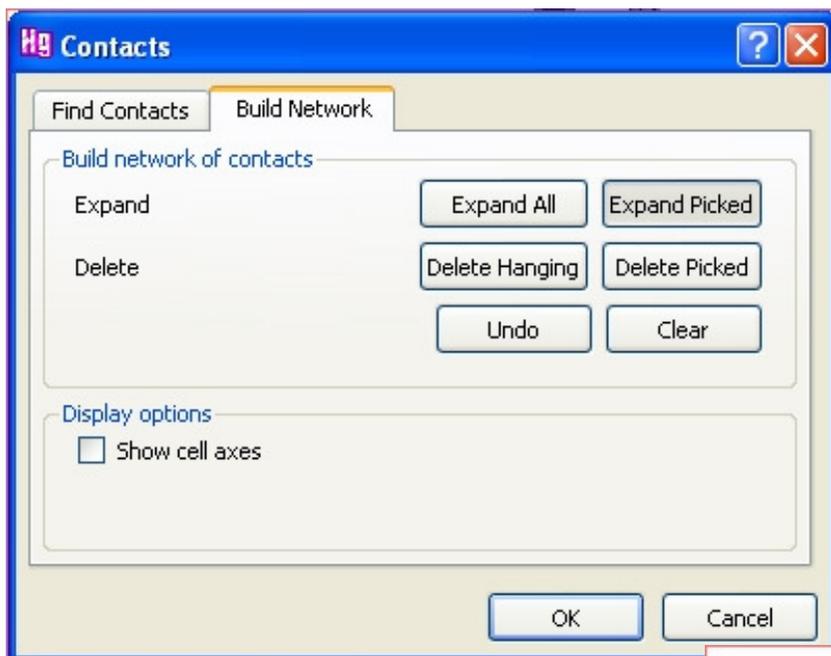
Click on a red contact to see the whole molecule



# Visualización molecular. Mercury y RasMol

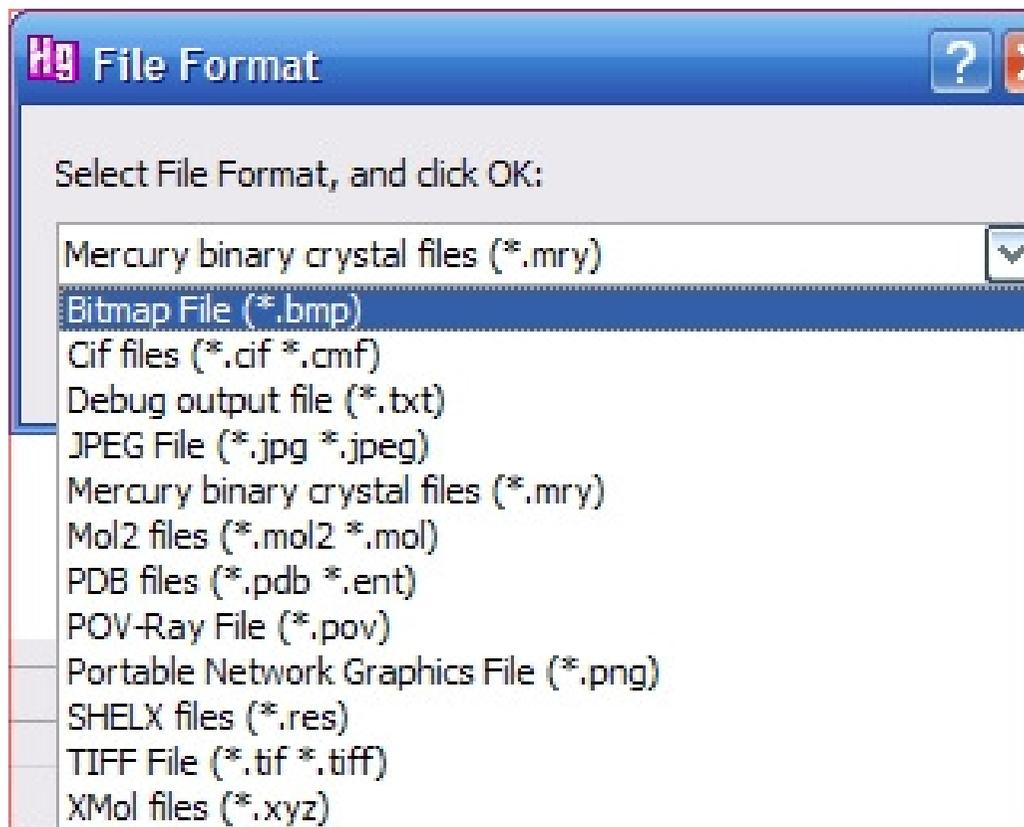
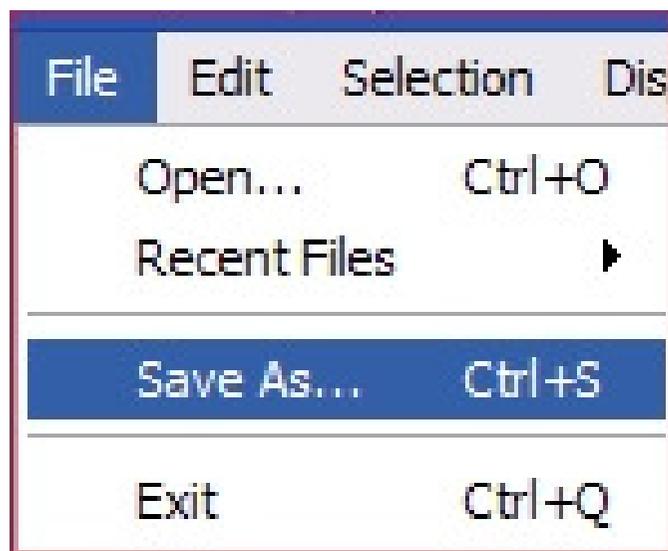


# Visualización molecular. Mercury y RasMol



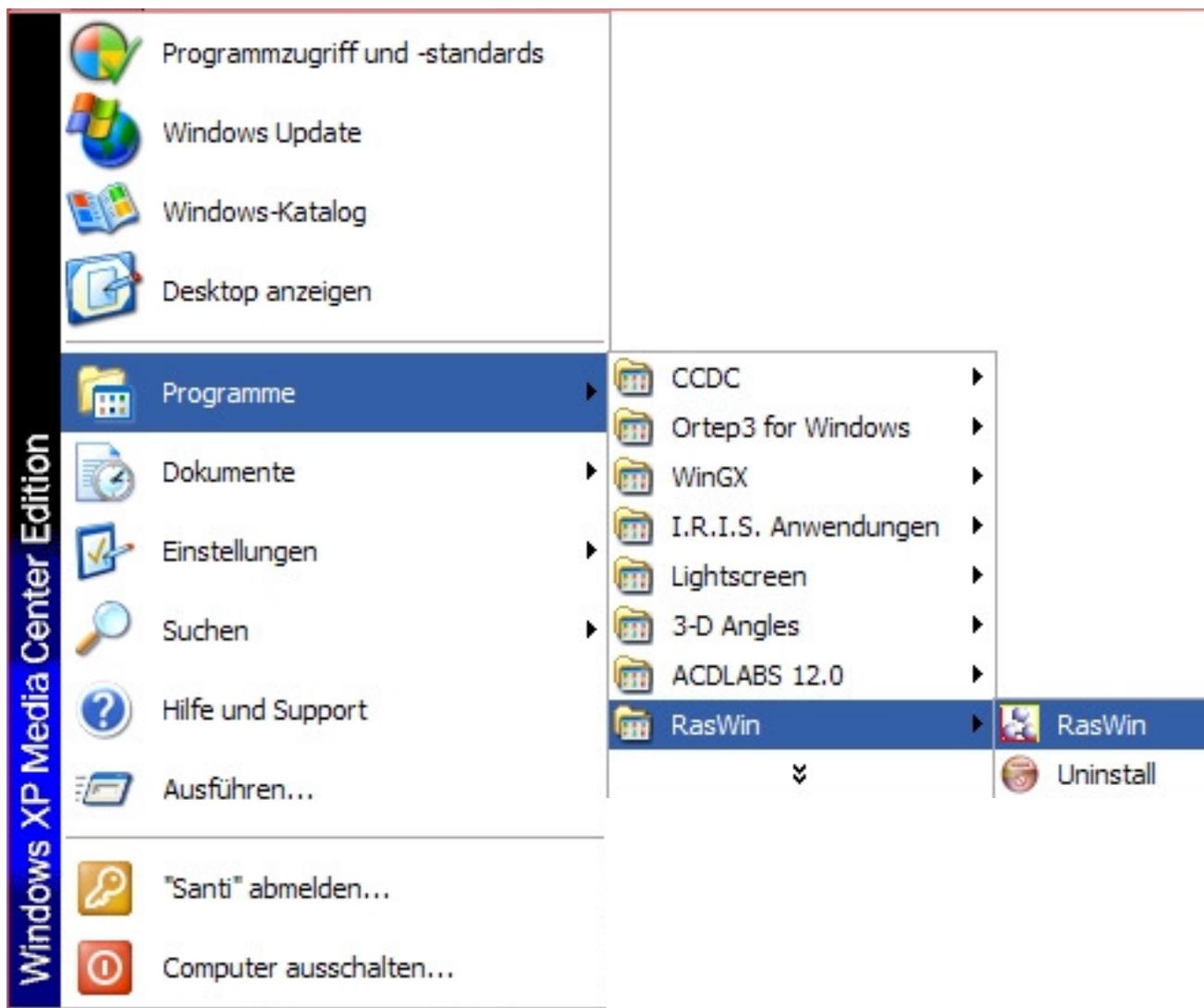
# Visualización molecular. Mercury y RasMol

- Mercury. Exportar a otros formatos y en imágenes



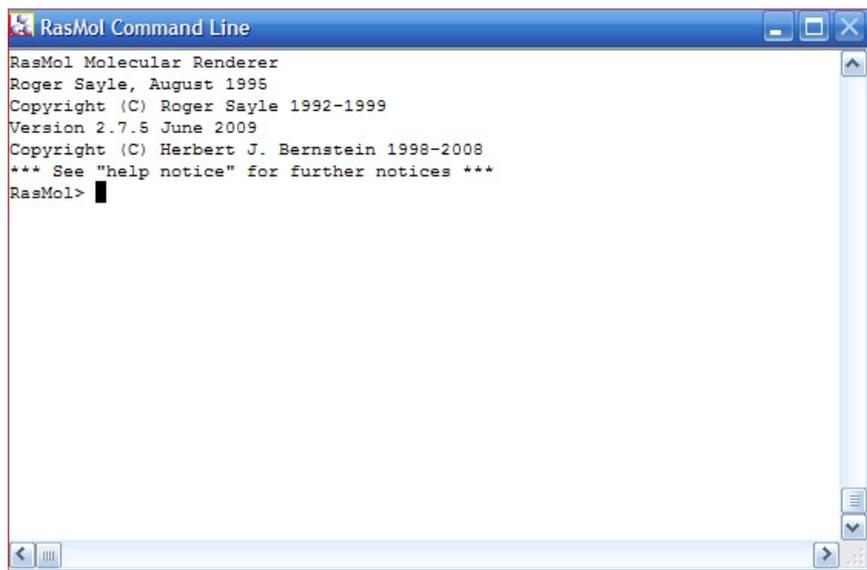
# Visualización molecular. Mercury y RasMol

- RasMol

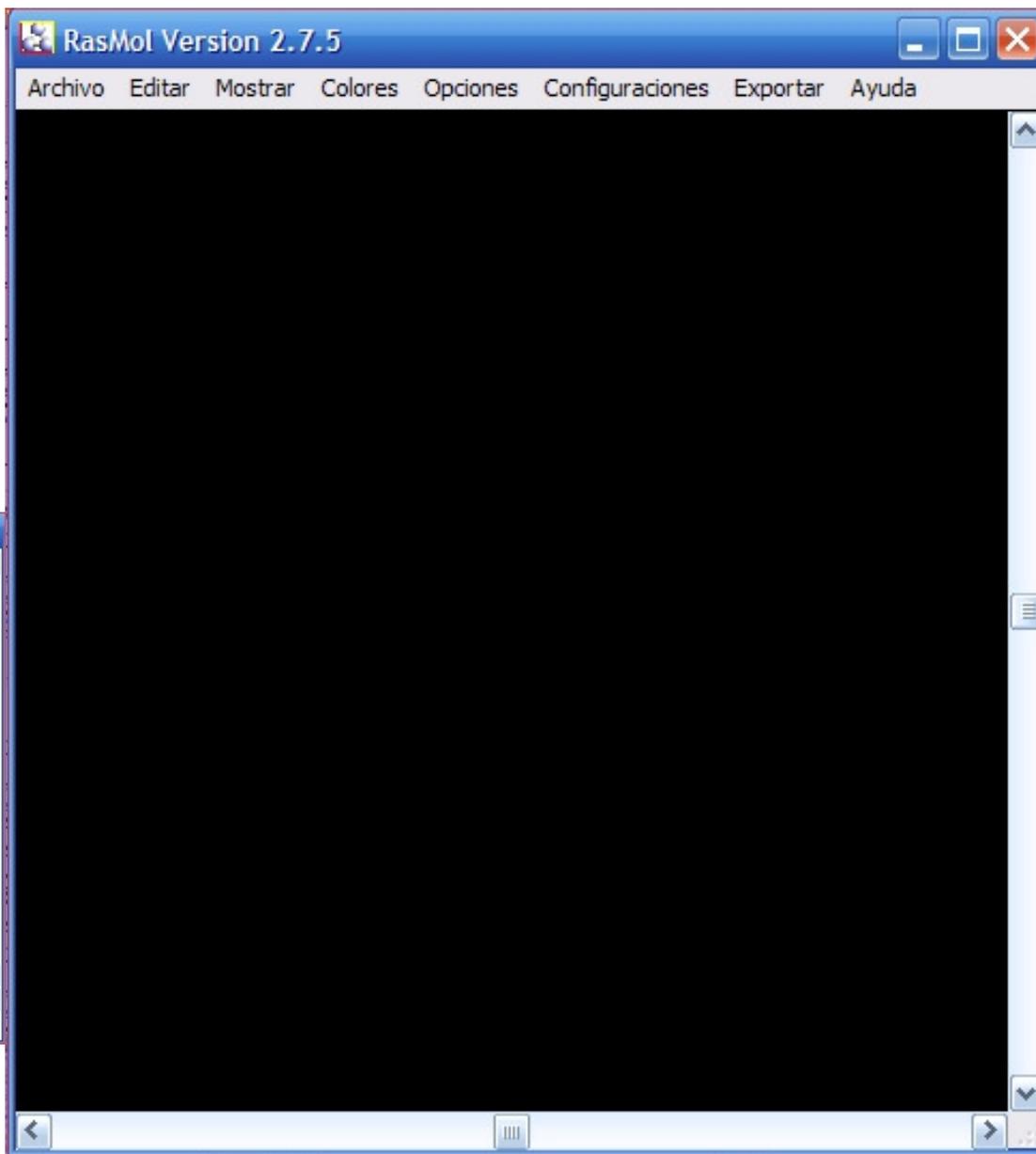


# Visualización molecular. Mercury y RasMol

- RasMol

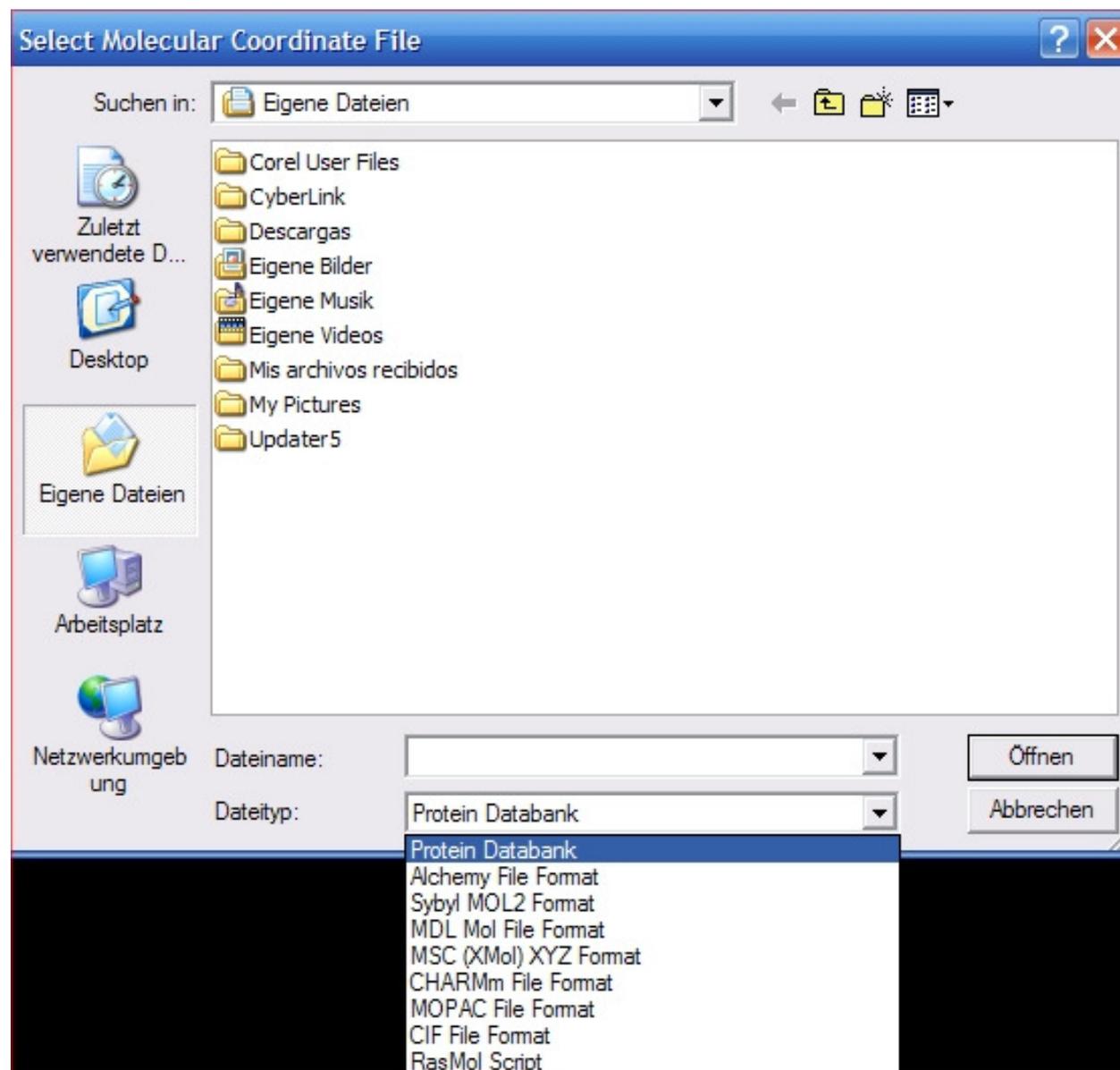
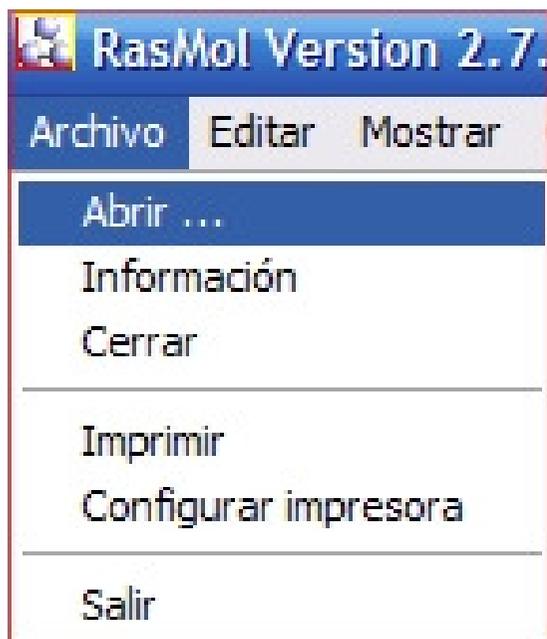


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RasMol Command Line
RasMol Molecular Renderer
Roger Sayle, August 1995
Copyright (C) Roger Sayle 1992-1999
Version 2.7.5 June 2009
Copyright (C) Herbert J. Bernstein 1998-2008
*** See "help notice" for further notices ***
RasMol>
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# Visualización molecular. Mercury y RasMol

- RasMol



# Visualización molecular. Mercury y RasMol

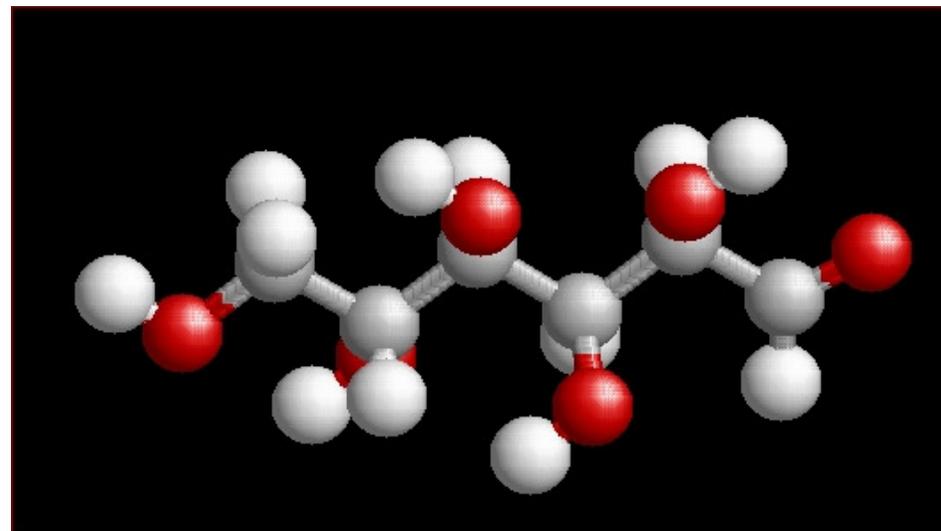
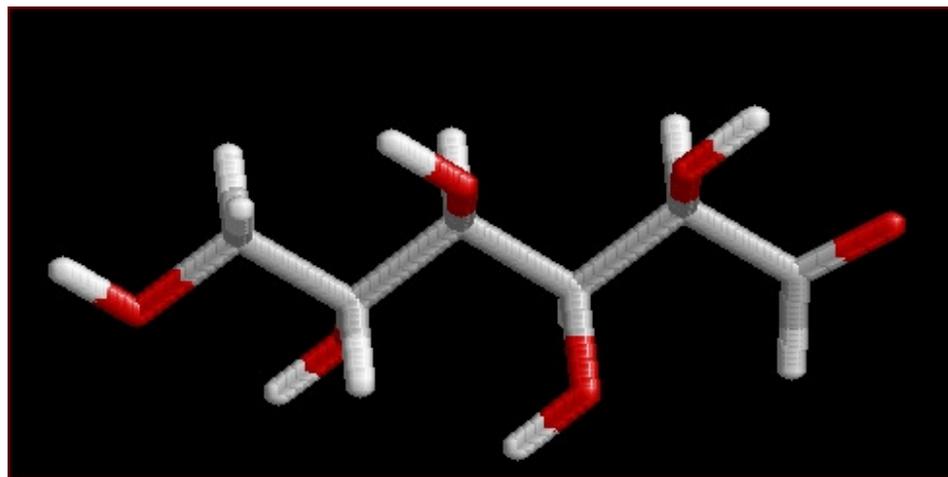
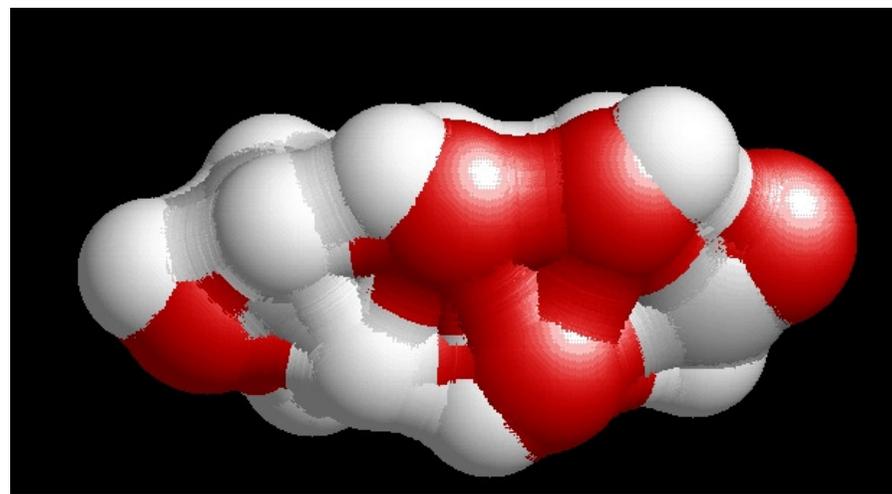
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- RasMol. Glucosa



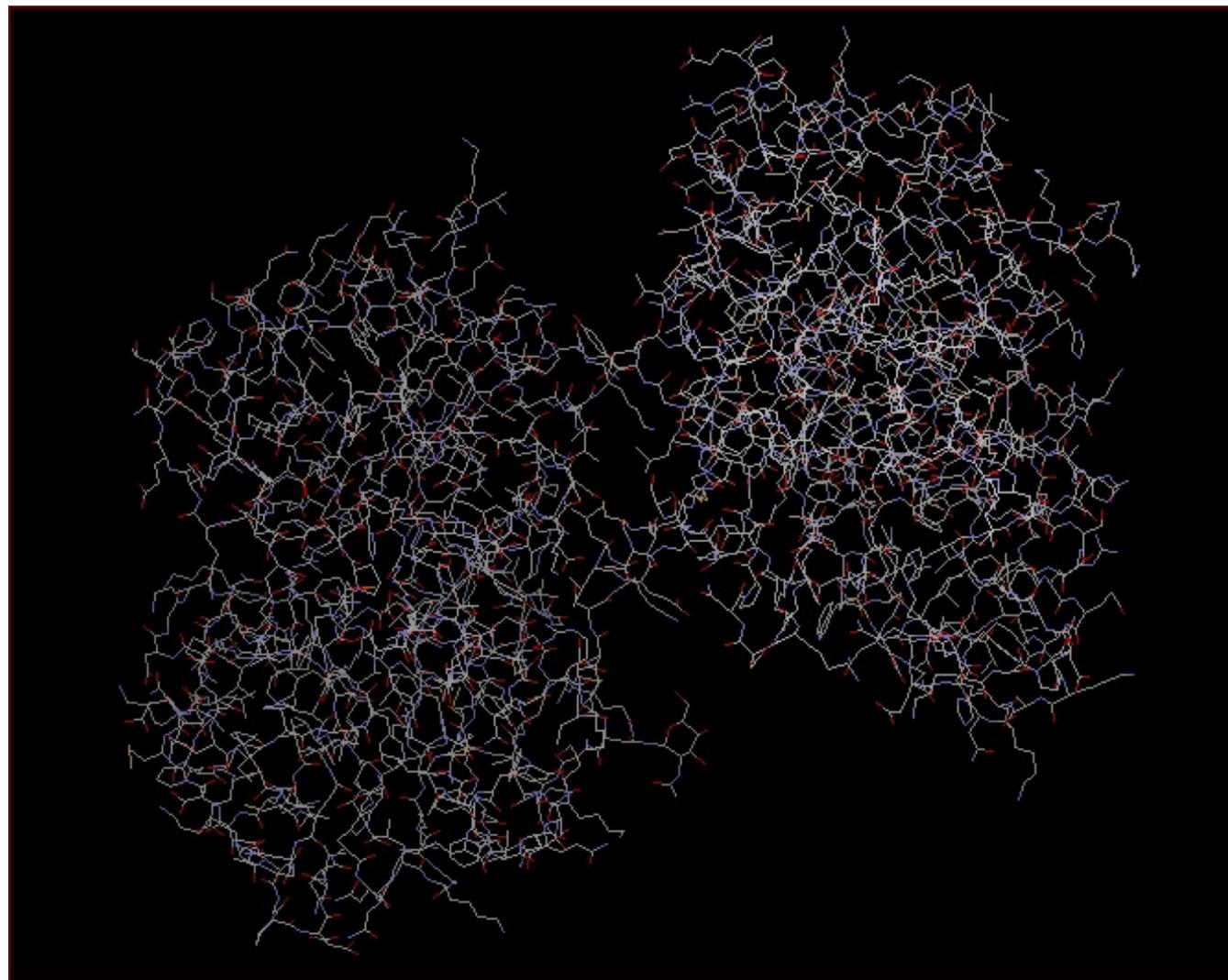
# Visualización molecular. Mercury y RasMol

- RasMol. Glucosa



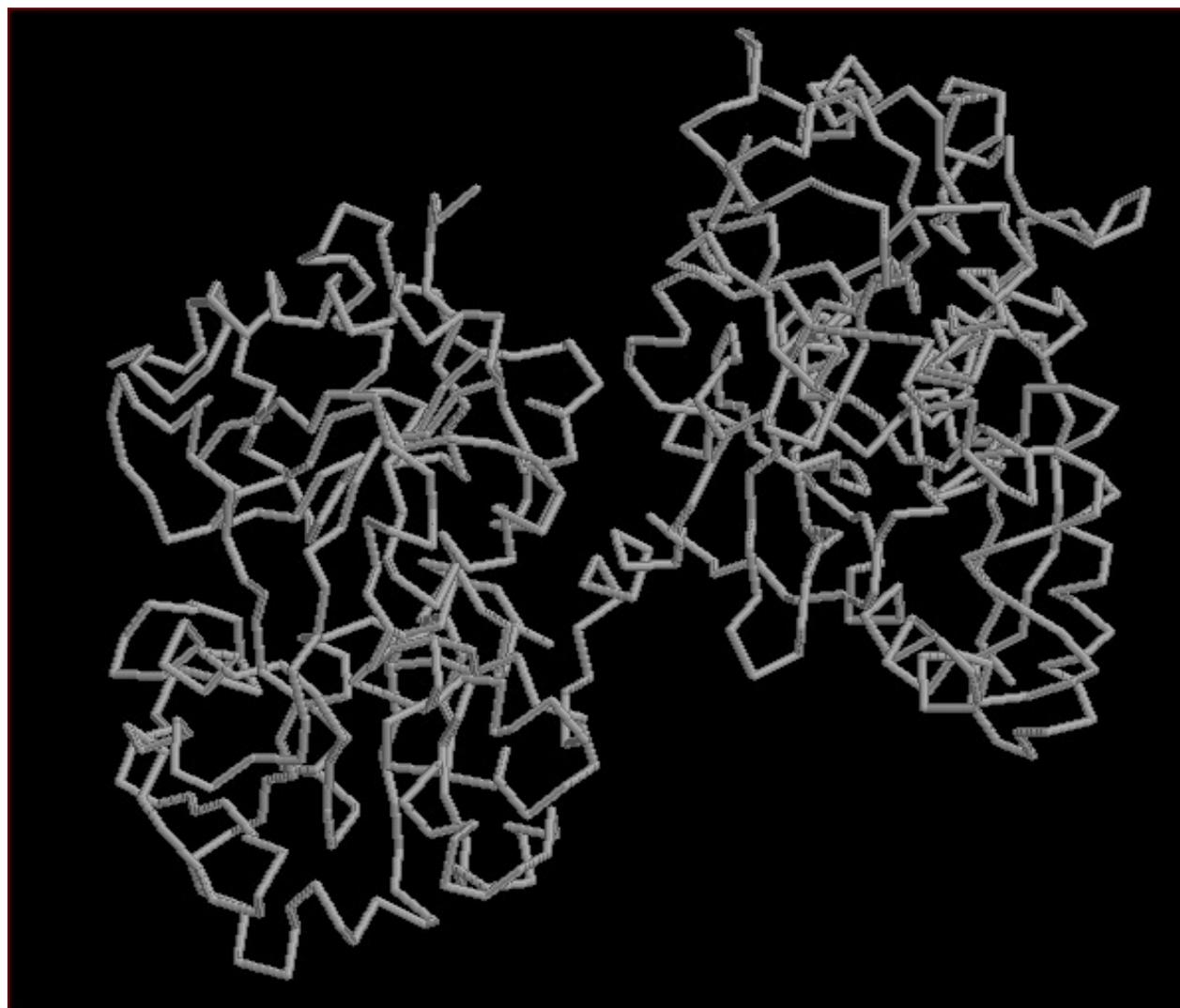
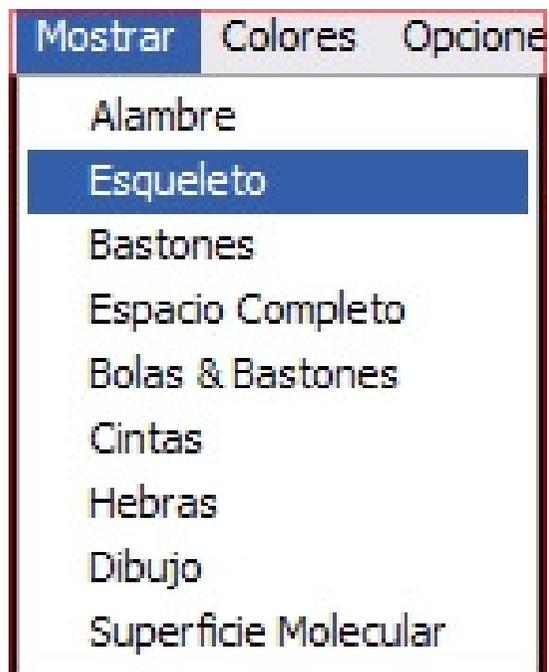
# Visualización molecular. Mercury y RasMol

- RasMol. Transferrina



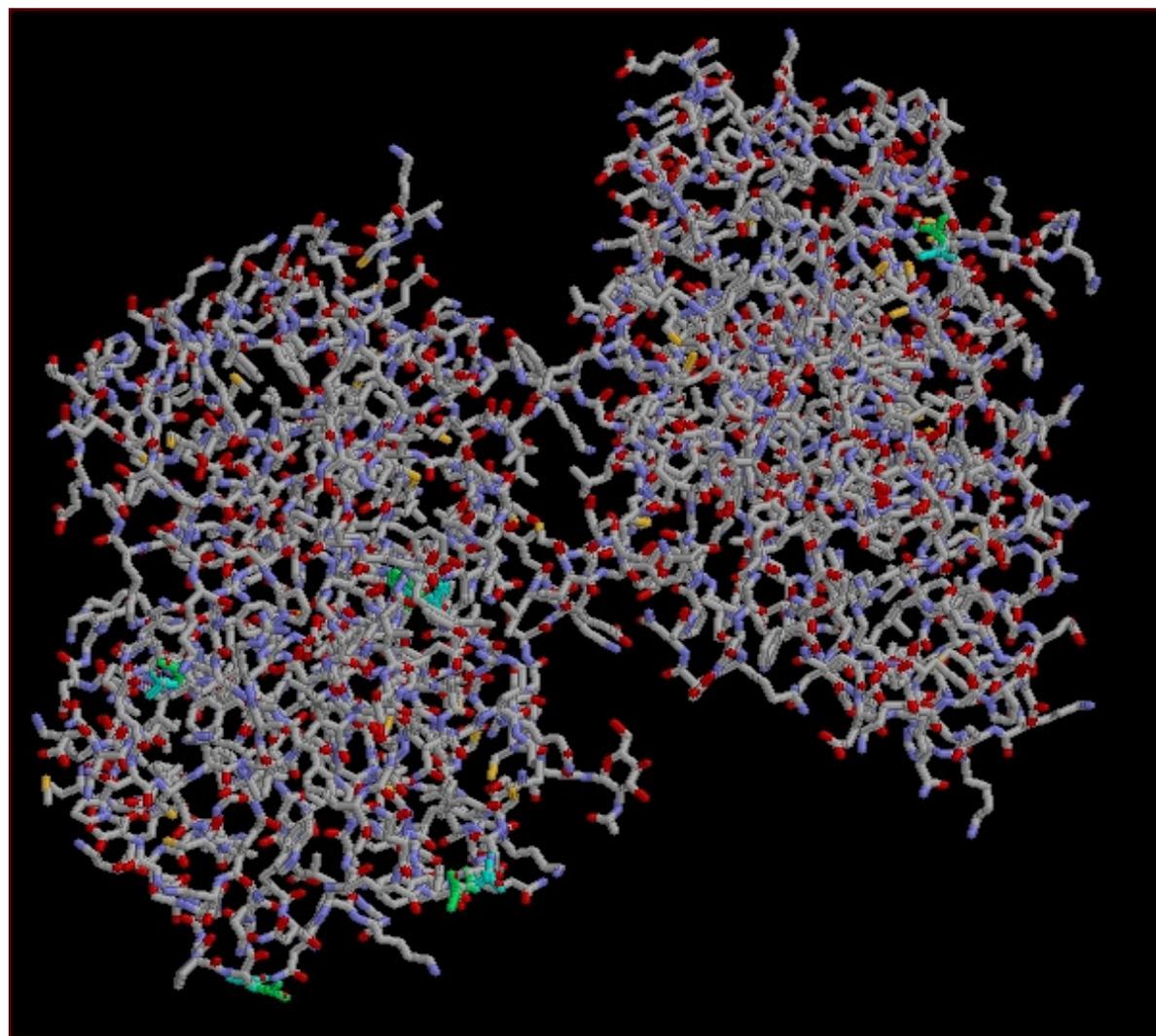
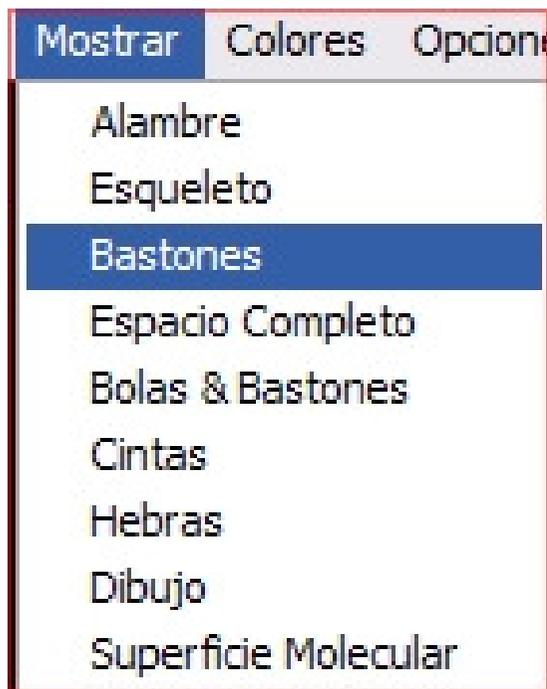
# Visualización molecular. Mercury y RasMol

- RasMol. Transferrina



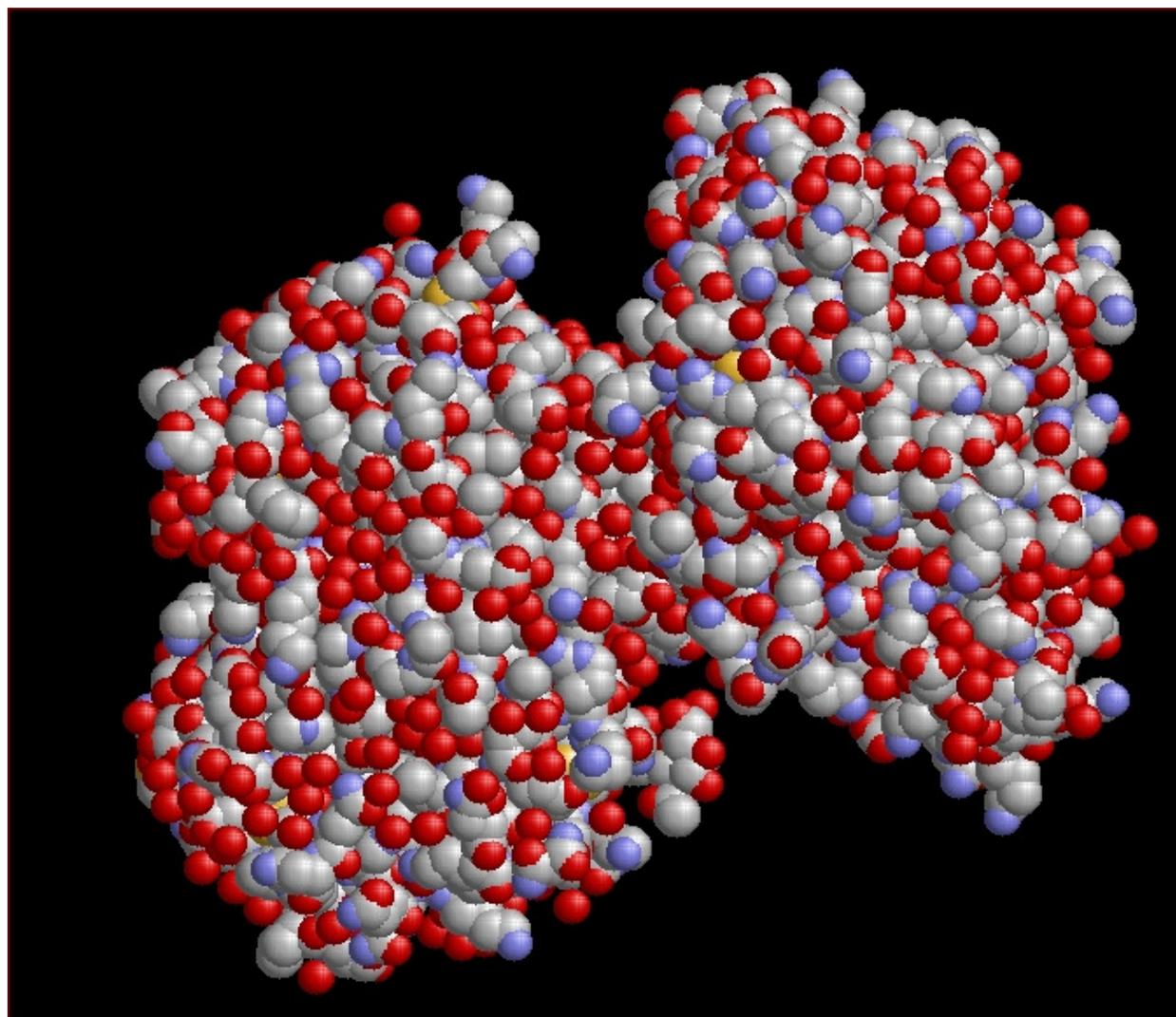
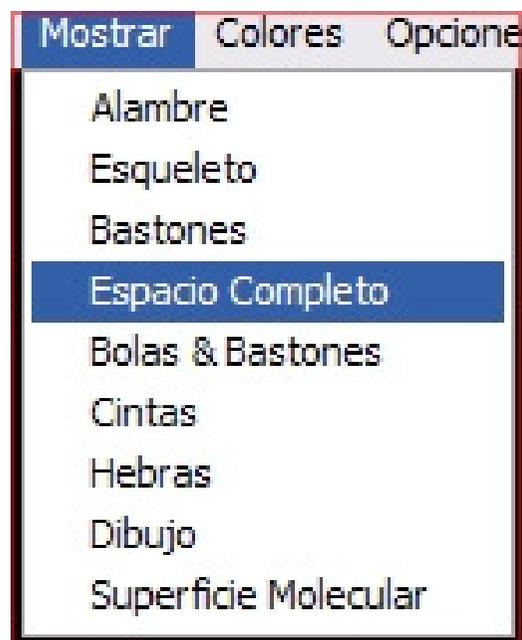
# Visualización molecular. Mercury y RasMol

- RasMol. Transferrina



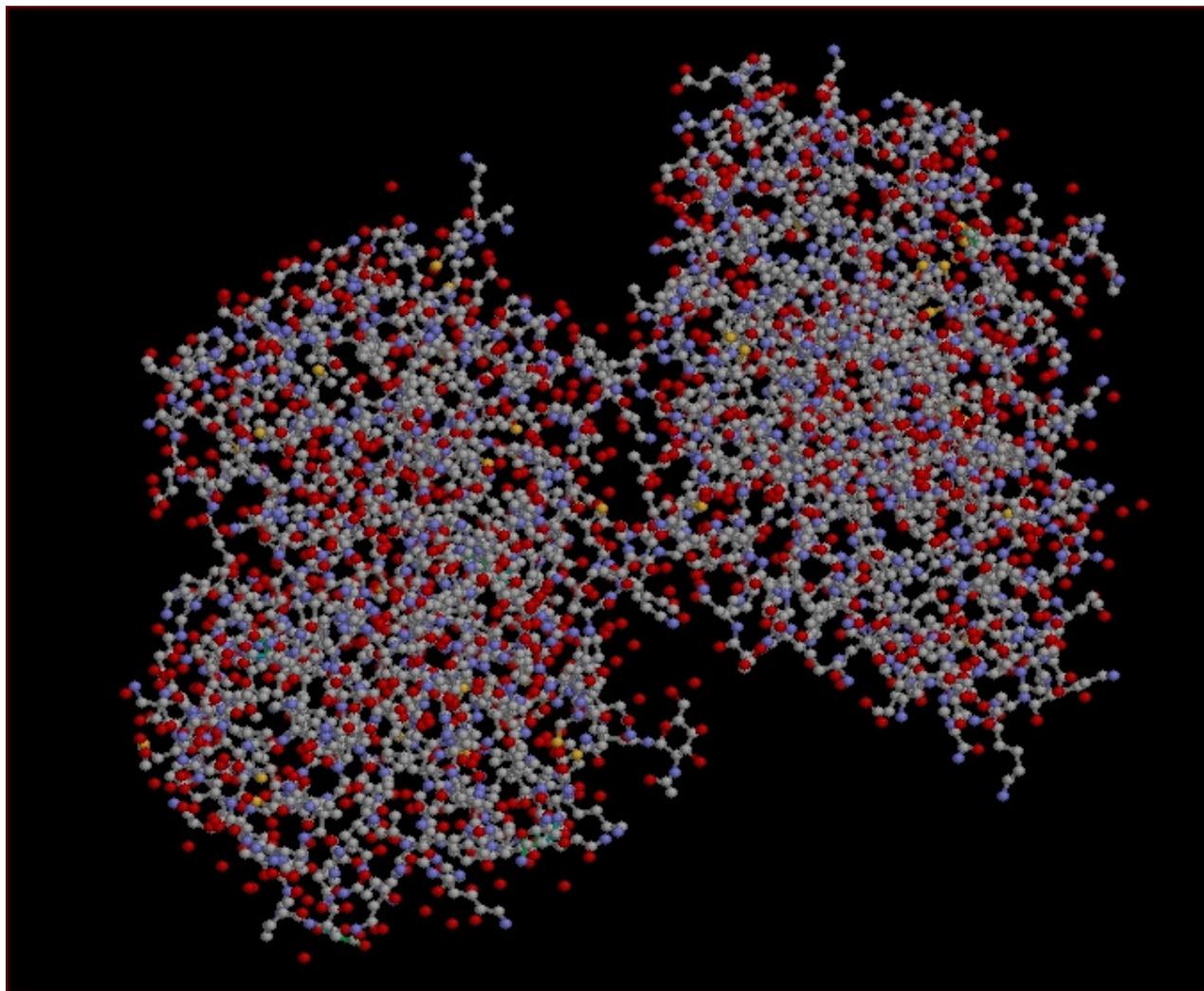
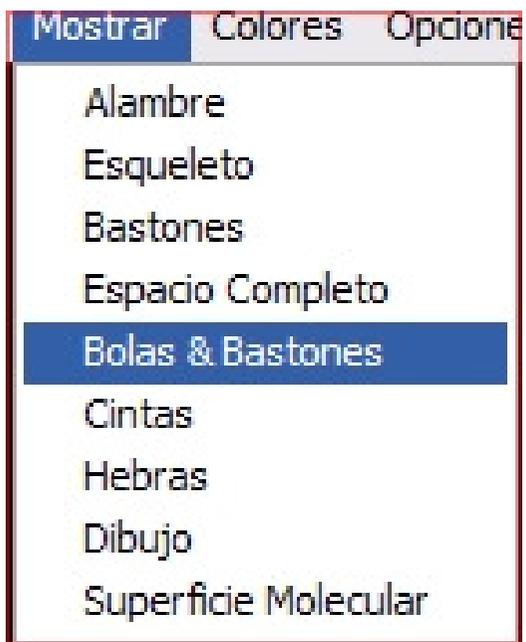
# Visualización molecular. Mercury y RasMol

- RasMol. Transferrina



# Visualización molecular. Mercury y RasMol

- RasMol. Transferrina



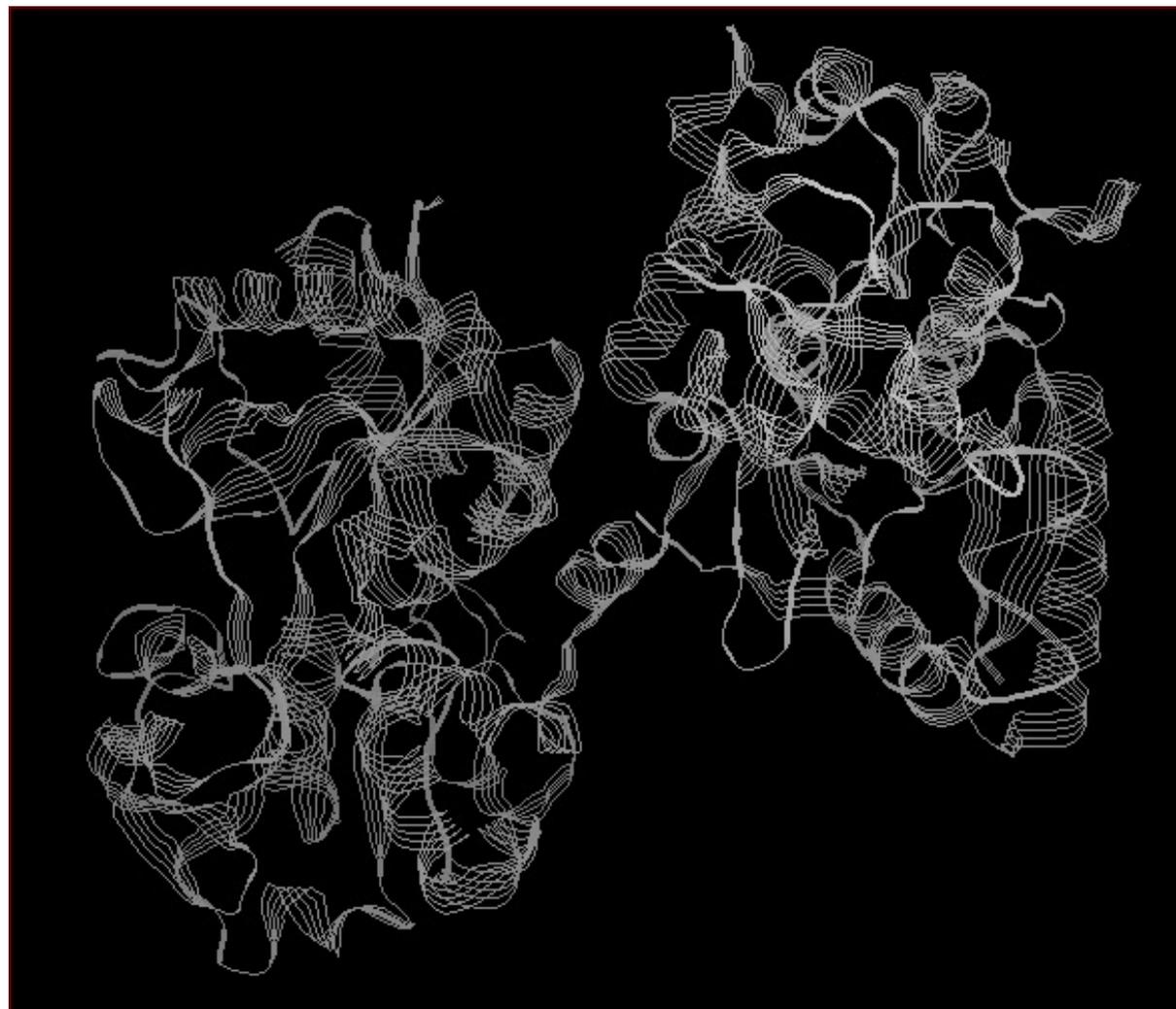
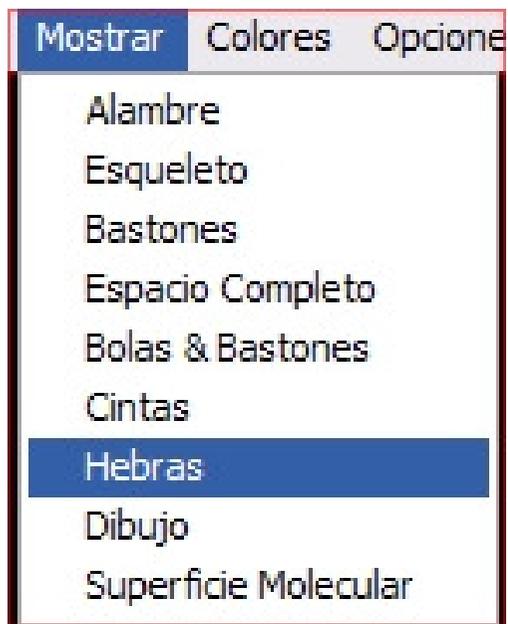
# Visualización molecular. Mercury y RasMol

- RasMol. Transferrina



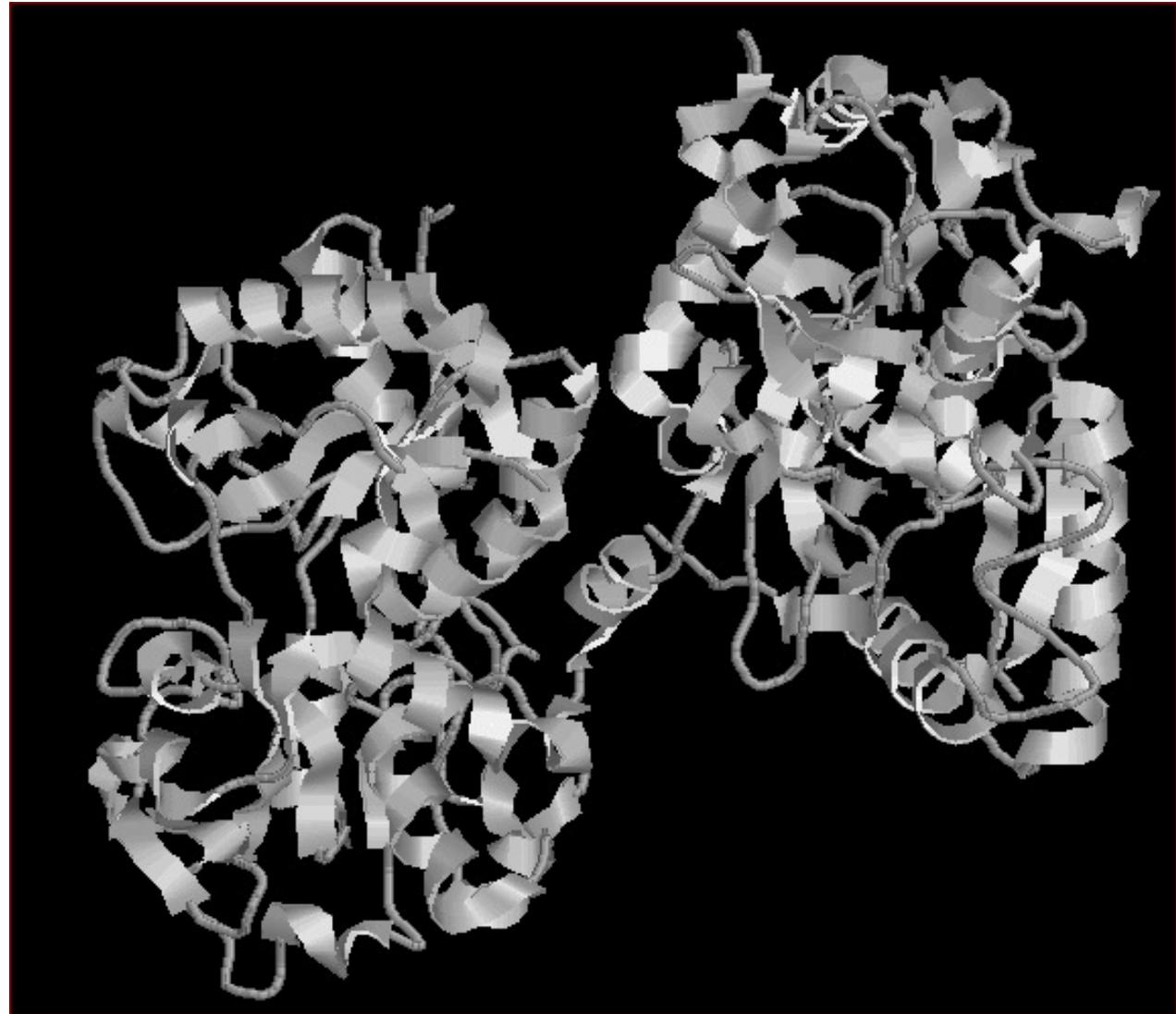
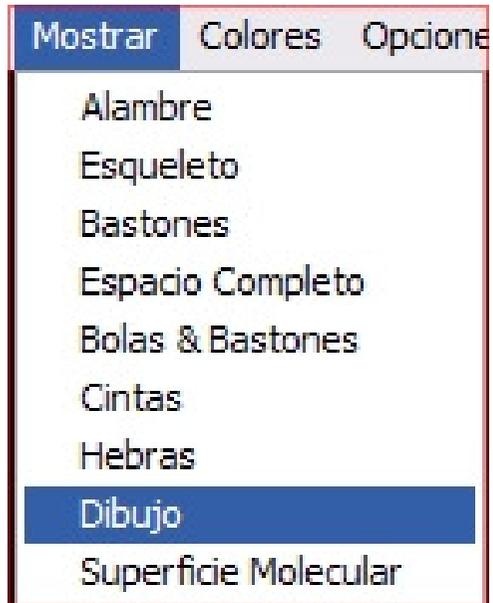
# Visualización molecular. Mercury y RasMol

- RasMol. Transferrina



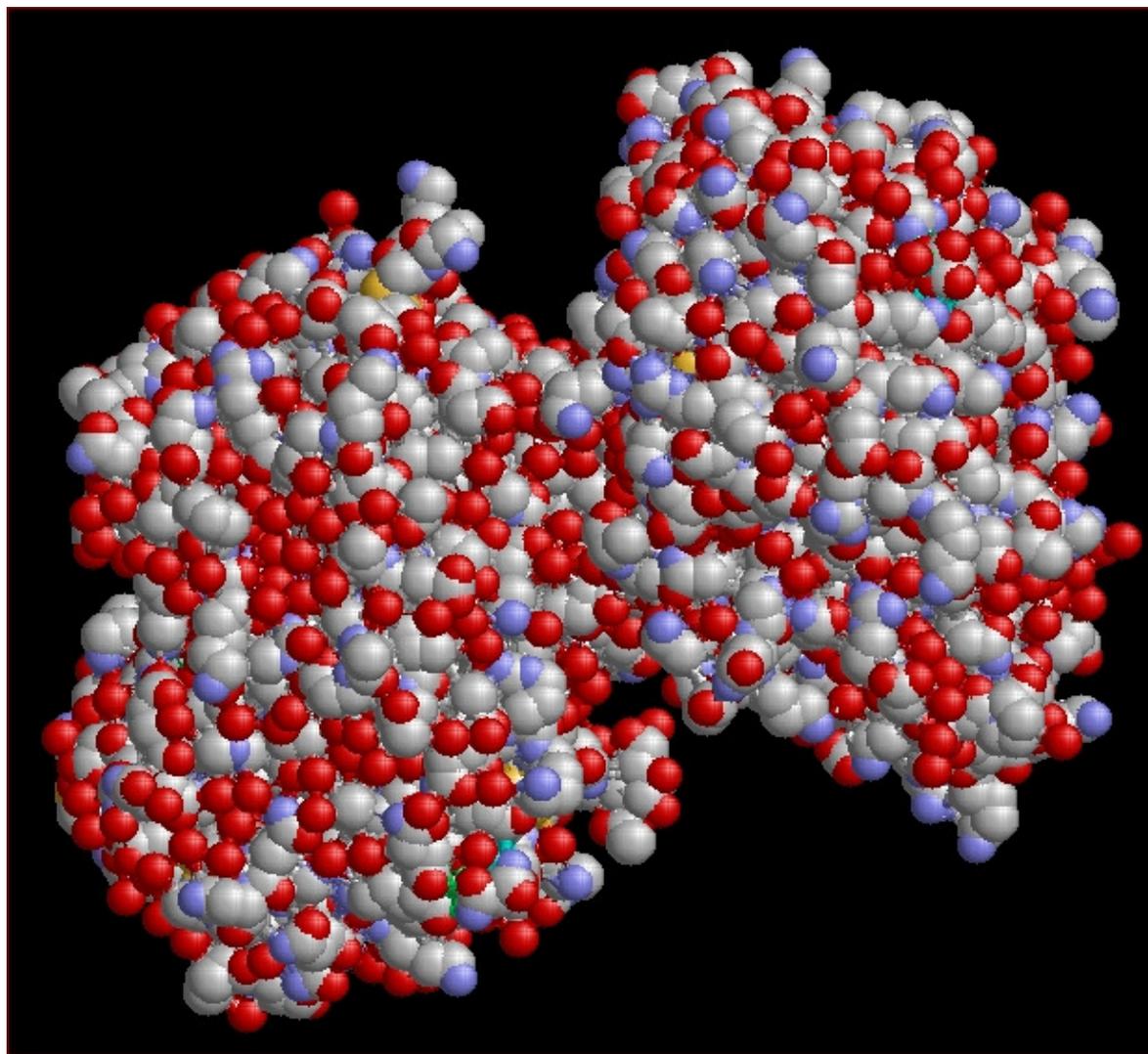
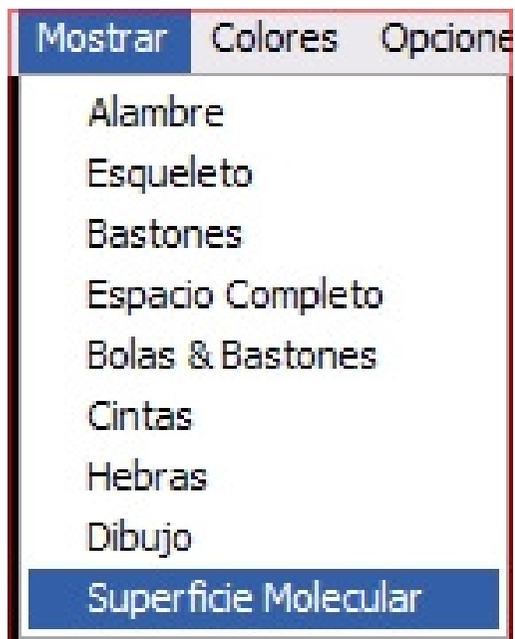
# Visualización molecular. Mercury y RasMol

- RasMol. Transferrina



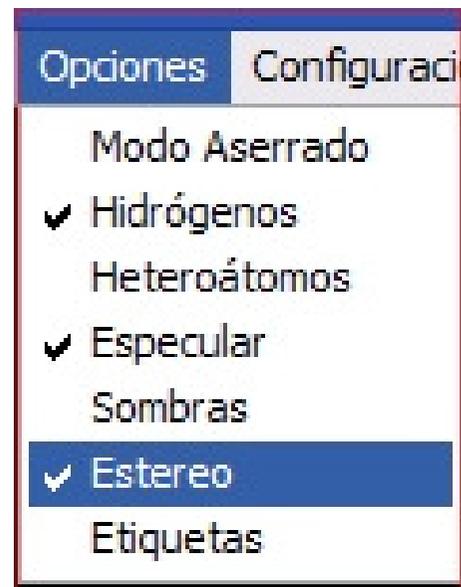
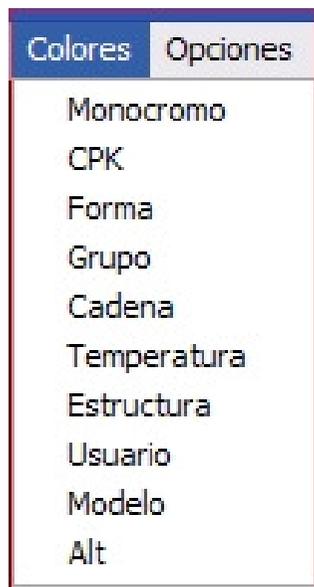
# Visualización molecular. Mercury y RasMol

- RasMol. Transferrina



# Visualización molecular. Mercury y RasMol

- RasMol. Glucosa



# Visualización molecular. Mercury y RasMol

- RasMol. Transferrin

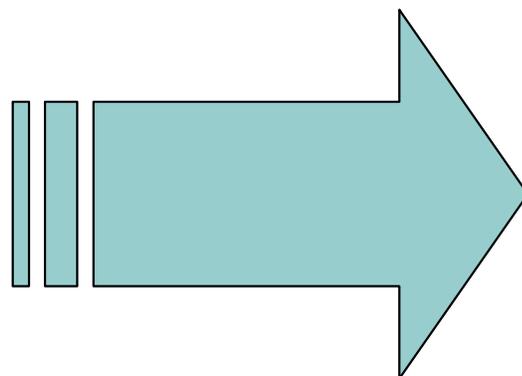
Configuraciones	Exportar
Desactivar elección	
Elegir identificación	
Elegir distancia	
Elegir monitor	
✓ Elegir ángulo	
Elegir torsiones	
Elegir etiqueta	
Elegir centro	
Elegir coordenadas	
Elegir enlace	
Girar enlace	
✓ Girar molécula	
Girar todo	

```
RasMol Command Line
24 atoms selected!
RasMol>
5254 atoms selected!
RasMol>
5772 atoms selected!
RasMol>
5254 atoms selected!
RasMol>
5772 atoms selected!
RasMol>
5772 atoms selected!
RasMol>
Atom #1: GLU389A.CA (2943)
RasMol>
Atom #2: LYS387A.CA (2930)
RasMol>
Atom #3: GLY388A.CA (2939)
Angle GLU389A.CA-LYS387A.CA-GLY388A.CA: 40.60

RasMol>
Atom #1: GLY388A.CA (2939)
RasMol>
```

# Visualización molecular. Mercury y RasMol

- RasMol.



**Cambio de formato,  
preparación de imágenes  
u otros que se pueden ver  
en otros programas de  
visualización molecular**