

Molècules en 3D: estructura i enllaç

XI Jornada de Física i Química a l'IEC «100 anys de la teoria de Lewis: l'enllaç químic a debat»

Dr. Roger Estrada Tejedor

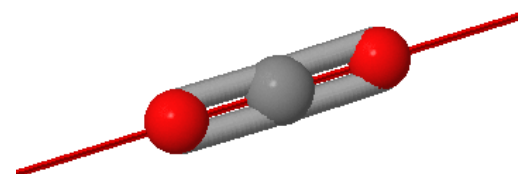
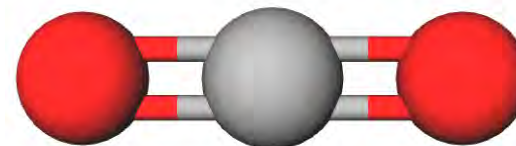
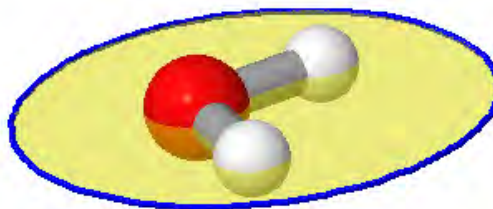
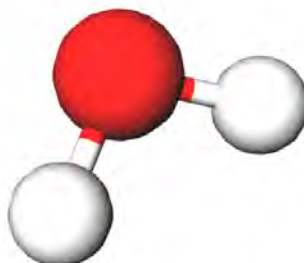
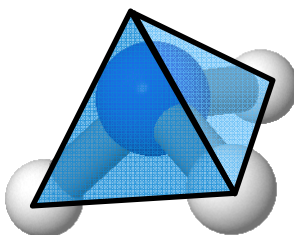
roger.estrada@iqs.url.edu



PERSONA CIÈNCIA EMPRESA
UNIVERSITAT RAMON LLULL

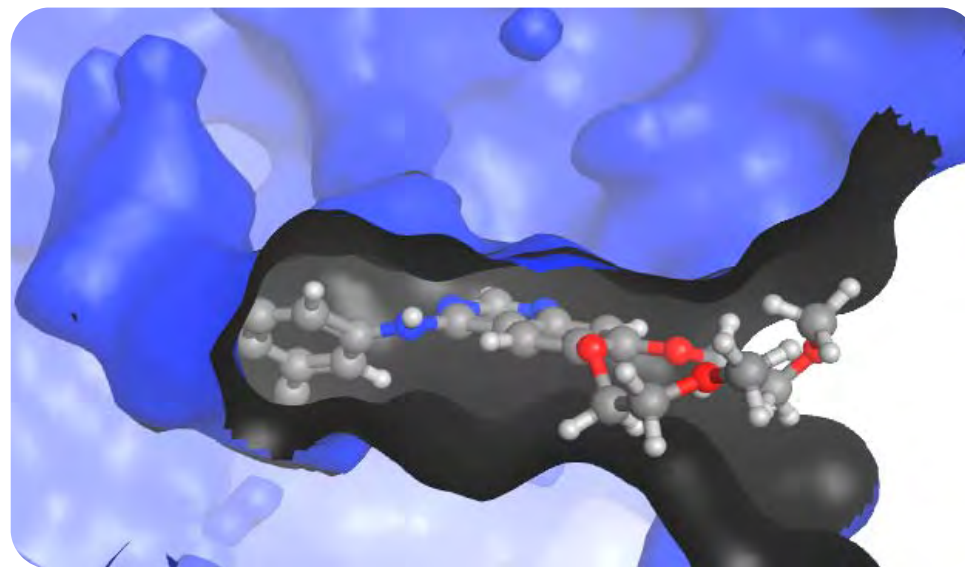
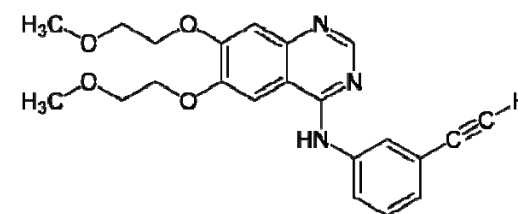
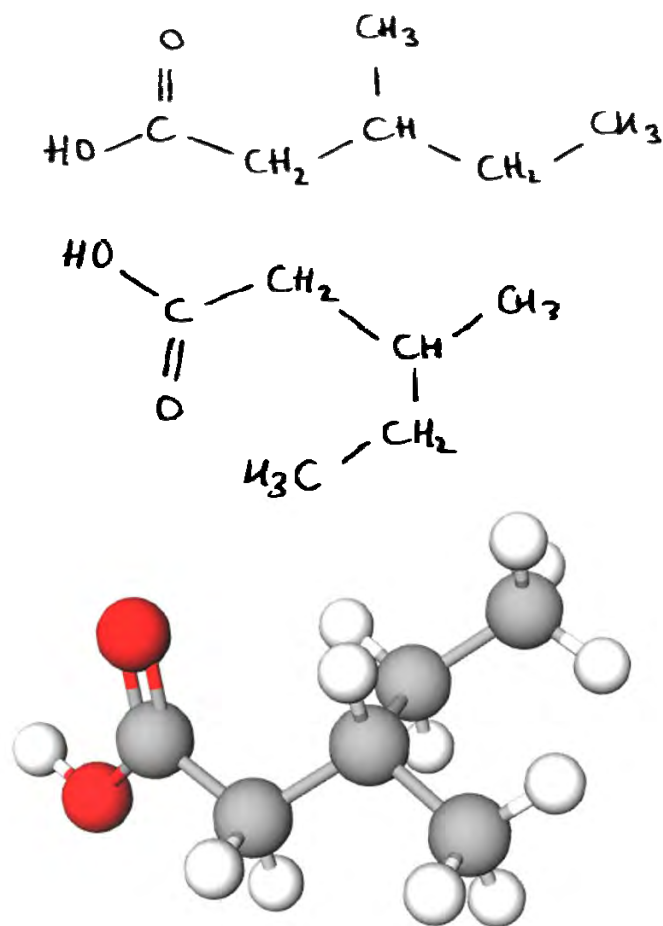
Del 2D al 3D... ¿per què?

- Quina és la geometria molecular?



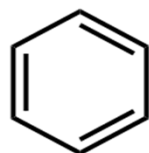
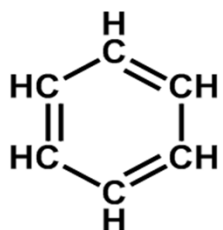
Del 2D al 3D... ¿per què?

- Les implicacions de les conformacions en molècules orgàniques

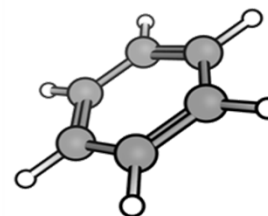
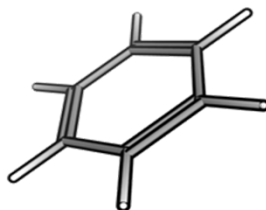


Representacions moleculars

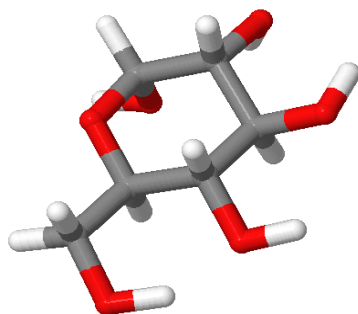
2D



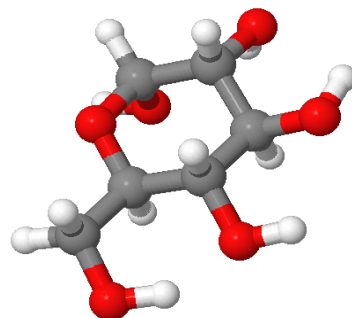
3D



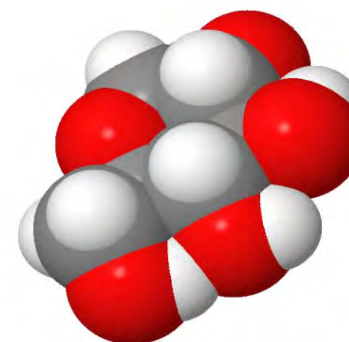
Jmol:



Varetes



Boles i varetes



Van der Waals

Distàncies, angles
Geometria de les hibridacions
Conformacions

Superfície
Forma molecular
Radi atòmic



On podem trobar informació?

PubChem

 **ChEMBL**

eMolecules®

ChemSpider
Search and share chemistry

DRUGBANK
Drug & Drug Target Database

 **ChemEd DL**
Chemical Education Digital Library **Models 360**

ZINC¹²

 **Compound SearchSM**

UniProt

 **MolView**  **AGPLv3**
Free Software
Free as in Freedom

RCSB PDB
PROTEIN DATA BANK

On podem trobar informació?



- Base de dades de molècules orgàniques
- Informació de >89 milions de compostos
- Estructura 3D optimitzades amb programes de modelització



Models 360

- Enfocat a l'ensenyament de la química
- Molècules inorgàniques, orgàniques i sòlids
- Estructura optimitzada i propietats validades pel seu ús educatiu
- Inclou algunes propietats: geometria, simetria, modes de vibració, orbitals moleculars,...



MolView



- Visualització d'estructures tridimensionals
- Fàcil interactivitat (conté un editor)
- Dades espectroscòpiques

PubChem

BioAssay ?

Compound ?

Substance ?

paracetamol

Go Limits Advanced

Nom o fórmula del compost químic

BioAssay Tools

Structure Search

3D Conformer Tools

Structure Clustering

Classification

Upload

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PubChem FTP

Try the PubChem Search Beta

New The PubChem Data Sources page is now updated. It helps you to find who provided what information in PubChem. [Read more...](#)

New PubChem Widgets 2.0f is released. It substantially updates all table-based widgets and classification widgets, while adding new capabilities and features. [Read more...](#)

more ...

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National Center for Biotechnology Information

NLM | NIH | HHS

Compound Summary for CID 1983

Download Print Share Help

PUBCHEM > COMPOUND > ACETAMINOPHEN

Acetaminophen

PubChem CID: 1983

Chemical Names: Acetaminophen; 4-Acetamidophenol; Paracetamol; 103-90-2; APAP; Tylenol

Molecular Formula: C8H9NO2 or HOC6H4NHCOCH3

Molecular Weight: 151.165 g/mol

InChI Key: RZVAJINKPMORJF-UHFFFAOYSA-N

Drug Information: [Drug Indication](#) [Therapeutic Uses](#) [FDA Orange Book](#) [FDA UNII](#)

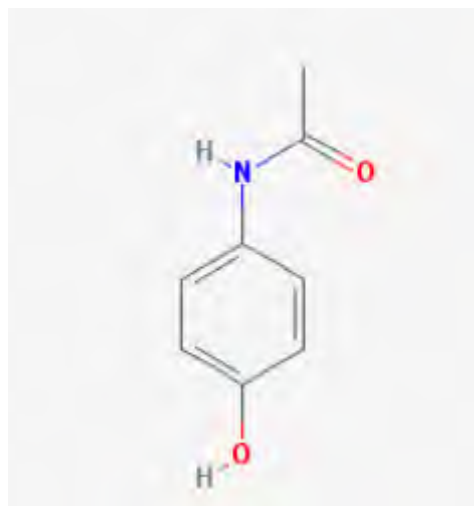
Safety Summary: [Laboratory Chemical Safety Summary \(LCSS\)](#)

- + Data used to display this page
- + 2D Structure
- + 3D Conformer
- + NCBI Linkout
- + Related Compounds with Annotation
- + Substances by Category
- + Chemical Vendors
- + Depositor Provided PubMed Citations
- + NLM Curated PubMed Citations
- + Depositor-Supplied Patent Identifiers
- + Protein Bound 3-D Structures

Modify Date: 2016-11-05; Create Date: 2004-09-16

+ Contents	«
1 2D Structure	^
2 3D Conformer	
3 Names and Identifiers	
4 Chemical and Physical Properties	
5 Related Records	
6 Chemical Vendors	
7 Drug and Medication Information	
8 Agrochemical Information	
9 Pharmacology and Biochemistry	
10 Use and Manufacturing	
11 Identification	
12 Safety and Hazards	
13 Toxicity	
14 Literature	»

2D Structure



3D Conformer



Names and Identifiers

IUPAC: N-(4-hydroxyphenyl)acetamide

InChI Key: RZVAJINKPMORJF-UHFFFAOYSA-N

Canonical SMILES: CC(=O)NC1=CC=C(C=C1)O

Molecular Formula: $C_8H_9NO_2$

ChemEd DL
Chemical Education Digital Library

Models 360

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[Molecules](#) [Solids](#)

[3D structure: Jmol](#) [Molecular Properties](#) [Images](#) [Export](#)

Sulfuric Acid H_2SO_4



Display

☐ Spin Molecule ☐ VdW radii

☐ Bond Length ☐ Bond Angles

☐ Atom Labels ☐ Partial charges ☒ Labels off

☐ Molecular Dipole ☐ Bond Dipoles

[Molecular Electrostatic Potential \(MEP\)](#)

[Molecular Vibrations](#)

[Symmetry Elements for Point Group \$C_2\$](#)

[Molecular Orbitals](#)

Related Molecules

[CH₃COOH](#)
Acetic Acid

[NH₃](#)
Ammonia

[NH₄^{\(+\)}](#)
Ammonium Ion

[HCO₃^{\(-\)}](#)
Bicarbonate Ion

[BCl₃](#)
Boron Trichloride

[Take a picture](#) [Reset](#)

[Popup window](#)

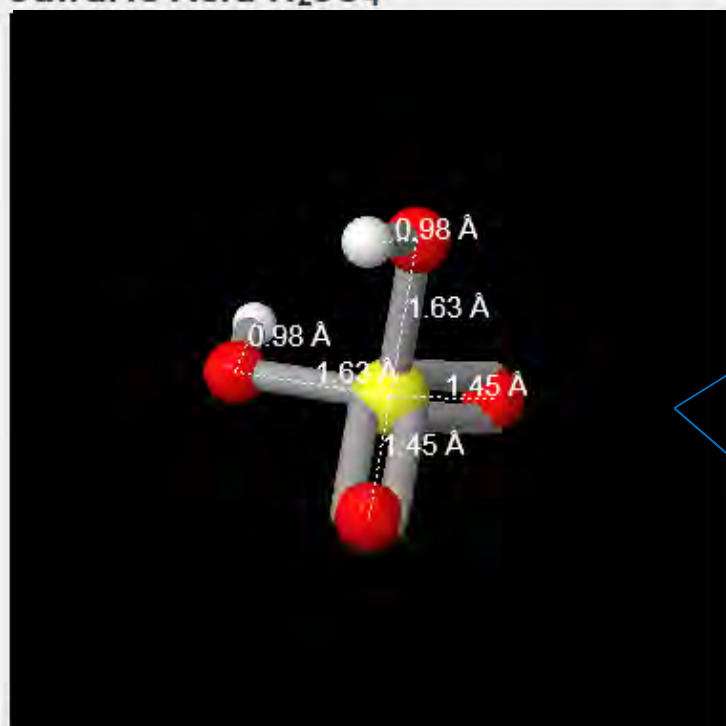
Nom o fórmula del
compost químic

Desar la imatge

Opcions de
visualització i
propietats moleculars

Suggestiments

Sulfuric Acid H₂SO₄



[Popup window](#)

[Take a picture](#)

[Reset](#)

Display

- ☐ Spin Molecule
- ☒ Bond Length
- ☐ Atom Labels
- ☐ Molecular Dipole
- ☐ VdW radii
- ☐ Bond Angles
- ☐ Partial charges
- ☐ Bond Dipole

[Molecular Electrostatic Potent](#)

[Molecular Vibrations](#)

[Symmetry Elements for Point](#)

[Molecular Orbitals](#)

*Distàncies
d'enllaç*

Related Molecules

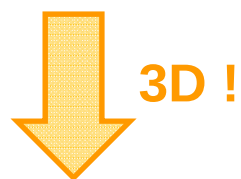
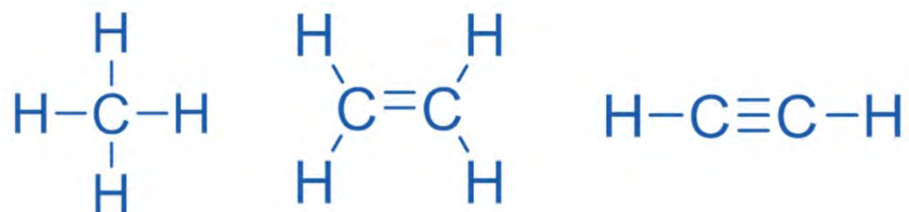


- model 2/17
- Configuracions
- Seleccions (110)
- Visualització
- Estil
- Color
- Superfícies
- Simetria
- Scenes
- Zoom
- Rotació
- Vibració
- Espectres
- Animació
- Mesures
- Defineix la tria
- Consola
- JavaScript Console
- Mostra
- Filtre
- Càlcul
- Idioma
- Quant a...

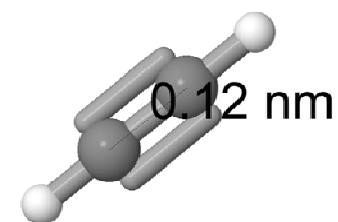
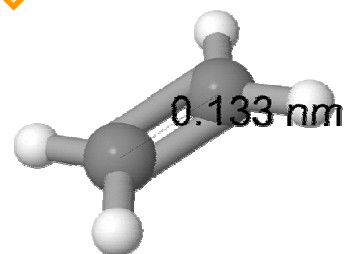
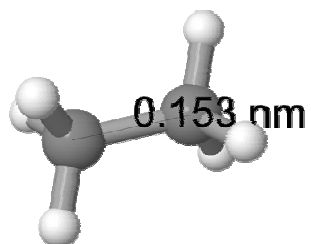
- ☒ Mostra les mesures
- Amb doble clic es comencen i acaben totes les mesures
- Feu clic per a mesurar la distància
- Feu clic per a mesurar l'angle
- Feu clic per a mesurar la torsió (angle dièdric)
- Feu clic per a mesurar la torsió (angle dièdric)
- Suprimeix les mesures
- Llista les mesures
- Unitats de distància en nanòmetres
- Unitats de distància en Angstroms
- Unitats de distància en picòmetres

Per exemple...

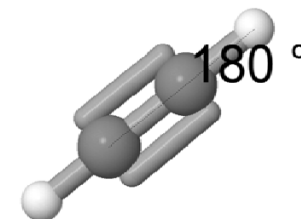
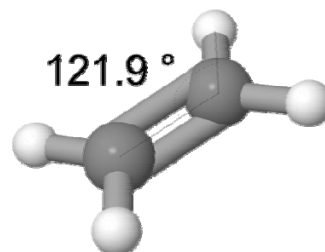
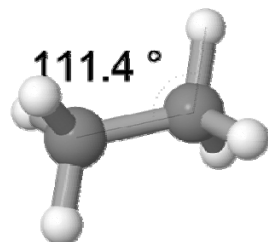
- Tots els enllaços C-C són iguals?



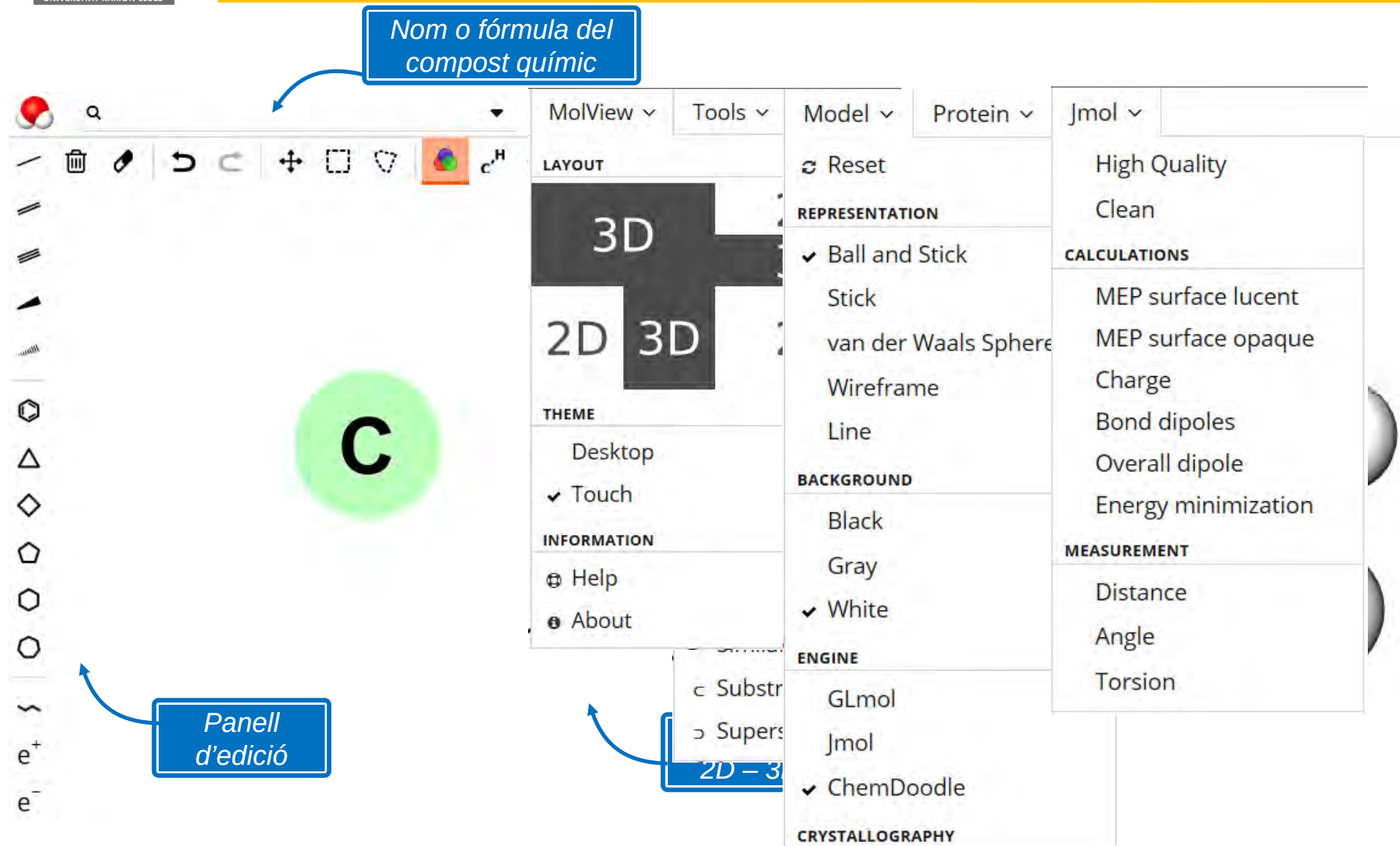
Distància C-C



Angle H-C-C



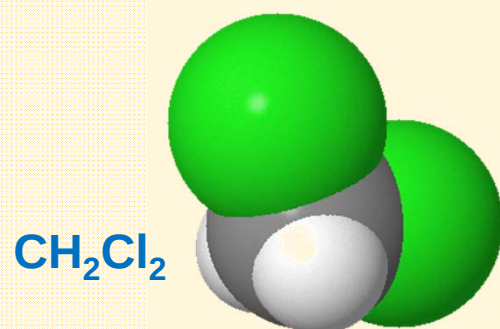
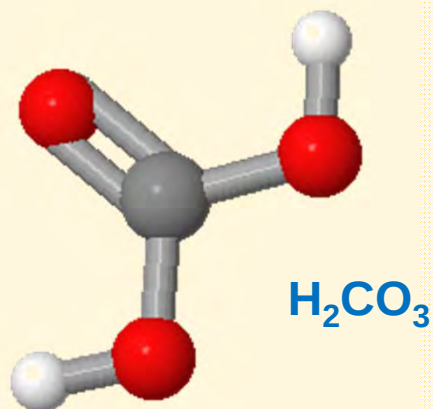
MolView



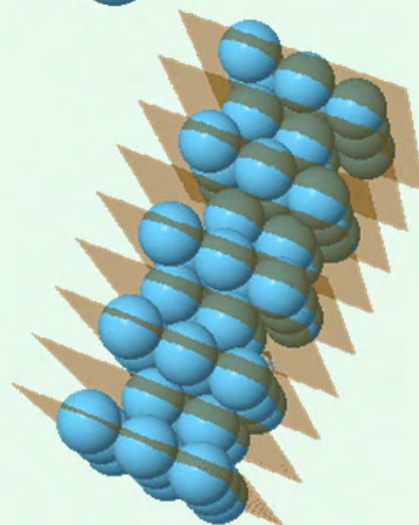
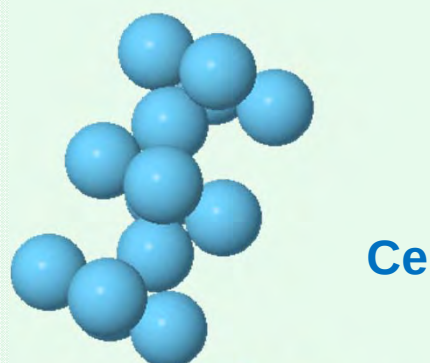
The screenshot shows the MolView web application interface. A central 3D model of a carbon atom (C) is displayed. The interface includes a top toolbar with various icons for file operations and editing. On the right, there are several dropdown menus for configuring the view: 'MolView', 'Tools', 'Model', 'Protein', and 'Jmol'. The 'Jmol' menu is currently open, showing options like 'High Quality', 'Clean', 'CALCULATIONS' (MEP surface, Charge, Bond dipoles, etc.), 'MEASUREMENT' (Distance, Angle, Torsion), and 'ENGINE' (GLmol, Jmol, ChemDoodle). A blue box with an arrow points to the top input field, labeled 'Nom o fórmula del compost químic'. Another blue box with an arrow points to the left toolbar, labeled 'Panell d'edició'. A third blue box with an arrow points to the '2D - 3D' toggle switch in the 'Model' dropdown menu.

Diferents tipus d'enllaç

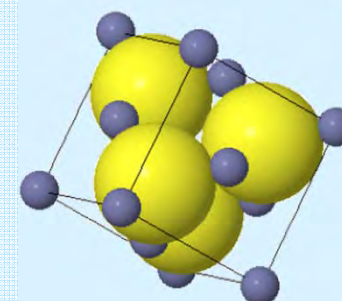
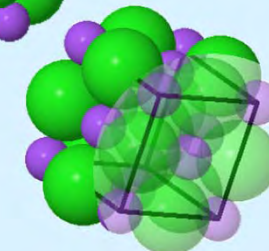
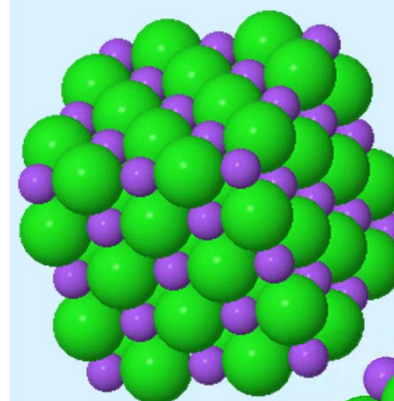
Molècules enllaç covalent



Estructures metàl·liques

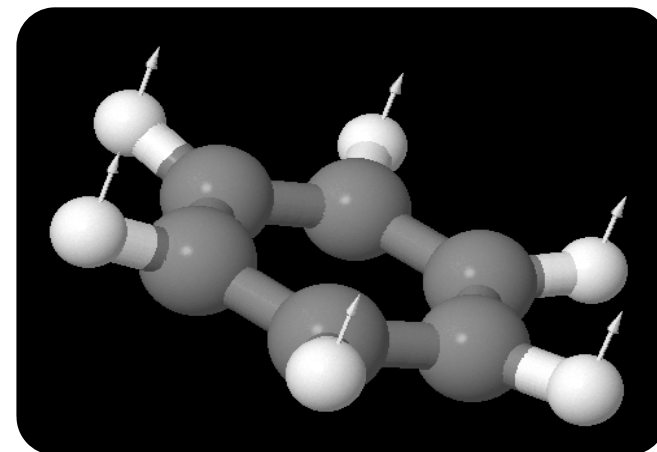
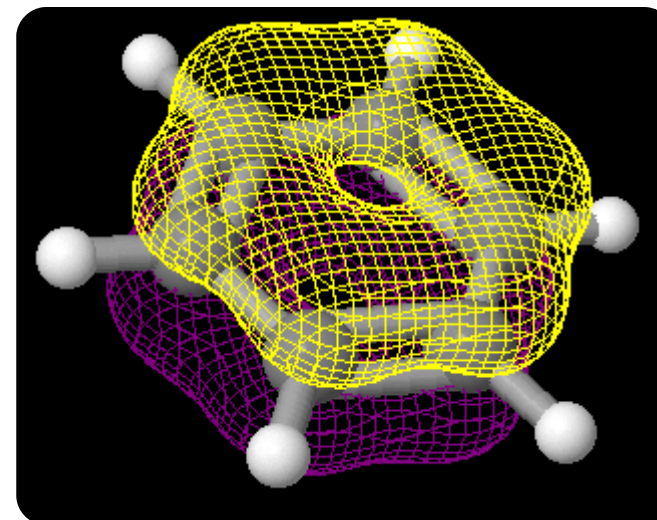
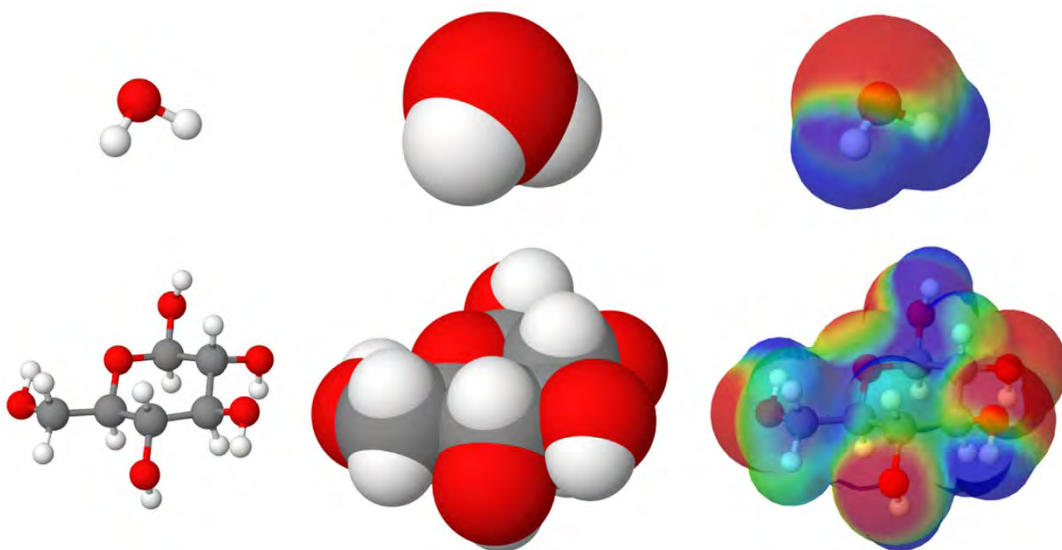


Estructures iòniques

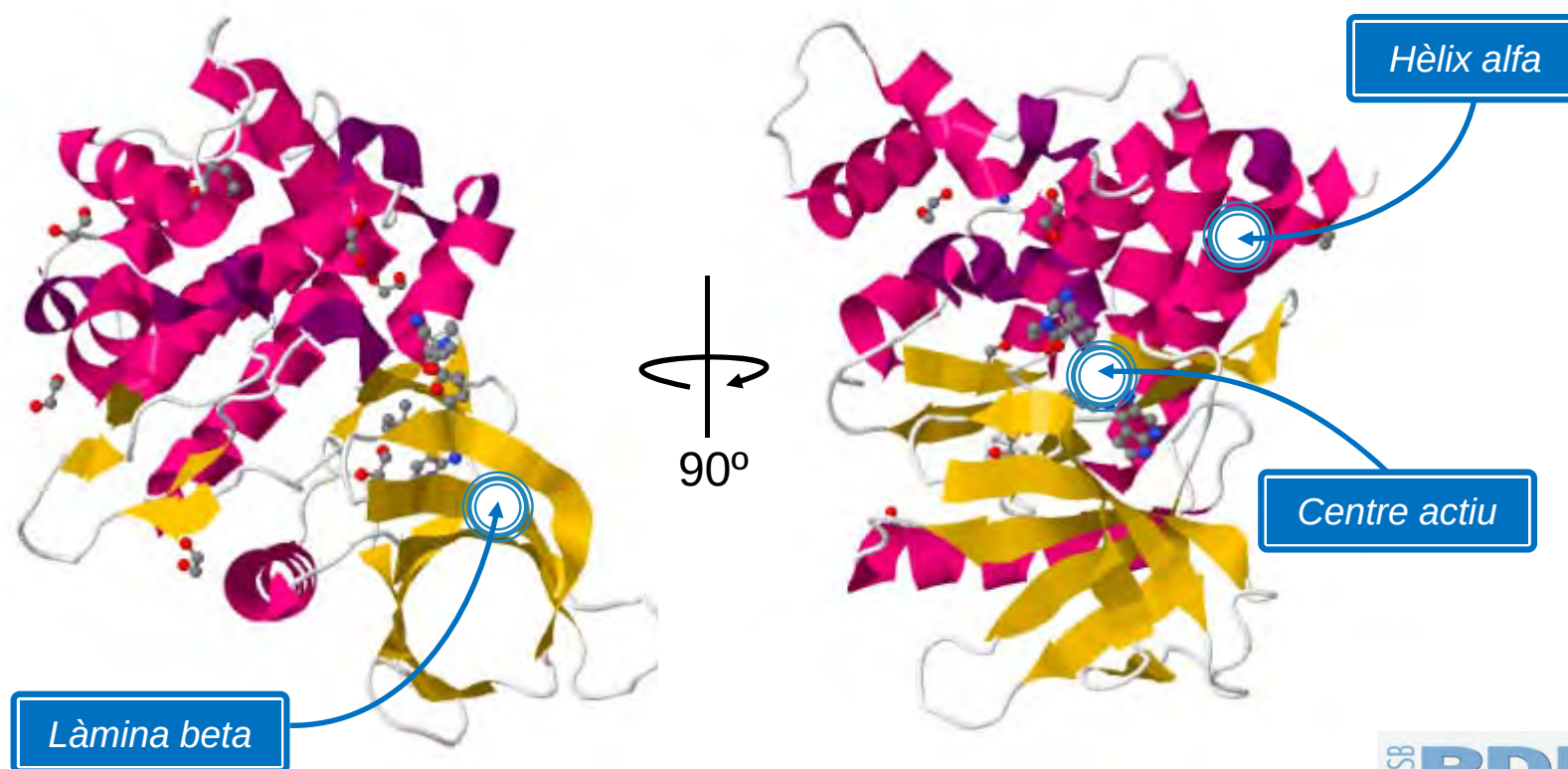


ZnS

- Superfícies
- Potencial electrostàtic emprant VdW
- Vibracions
- Orbitals moleculars



- Prenem d'exemple l'estructura de la proteïna JAK3...



RCSB **PDB**
PROTEIN DATA BANK

 **MolView** 
Free as in Freedom

Del 2D al 3D

ChemSpider
Search and share chemistry

ChEMBL

NCBI PDB
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DRUGBANK
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PubChem



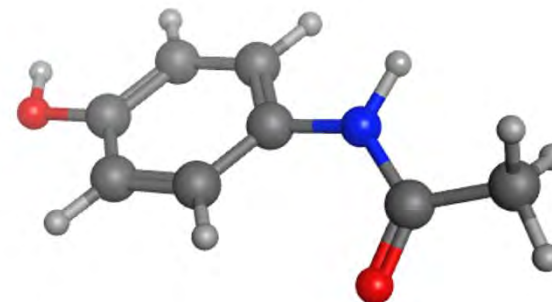
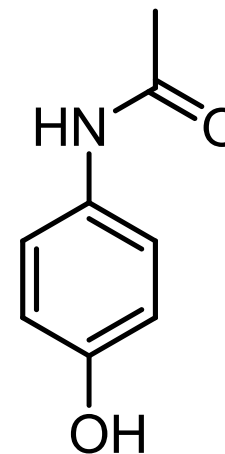
MolView

AGPLv3
Free as in Freedom



ChemEd DL
Chemical Education Digital Library

Models 360



Moltes gràcies per la seva atenció!

Dr. Roger Estrada Tejedor

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Agraïments: Dr. Jordi Cuadros, Dra. Laia Ros



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