Molècules en 3D: estructura i enllaç

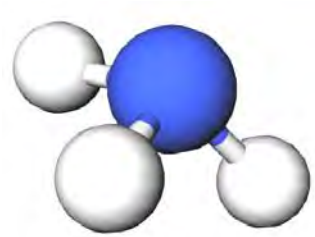
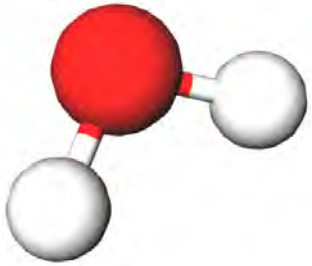
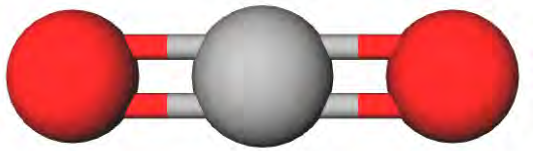
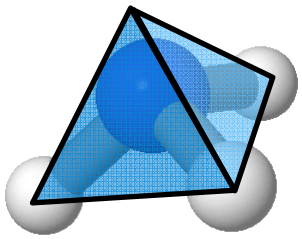
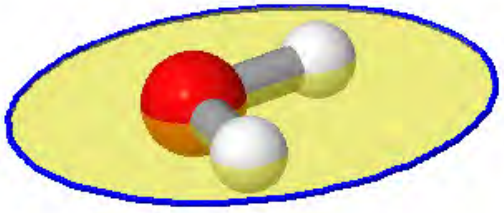
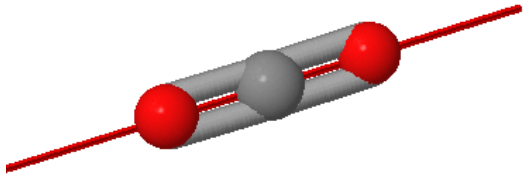
XI Jornada de Física i Química a l'IEC «100 anys de la teoria de Lewis: l'enllaç químic a debat»

Dr. Roger Estrada Tejedor

roger.estrada@iqs.url.edu

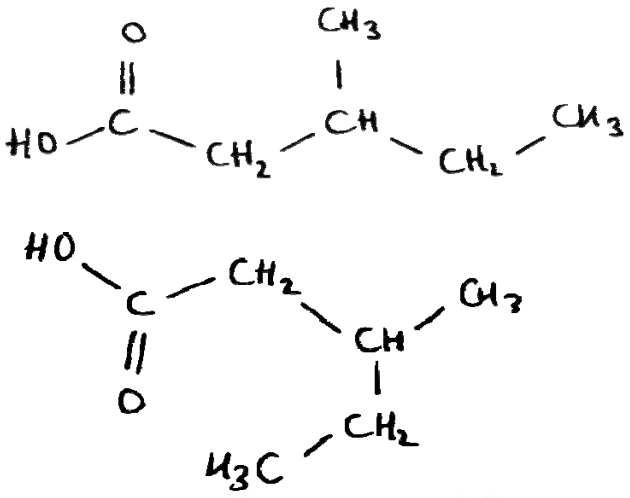
Del 2D al 3D... ¿per què?

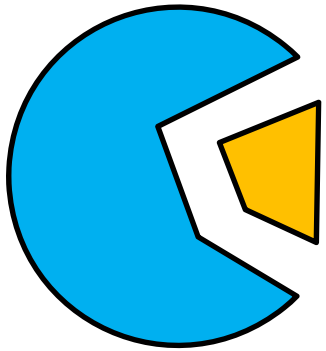
- Quina és la geometria molecular?

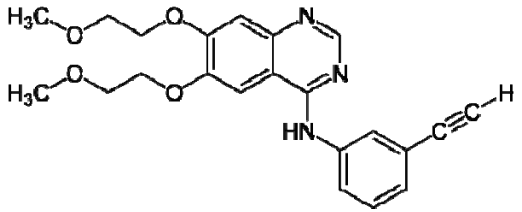
NH_3	H_2O	CO_2
		
		

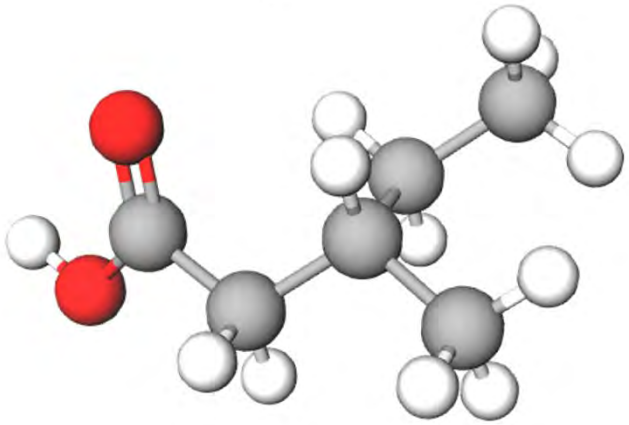
Del 2D al 3D... ¿per què?

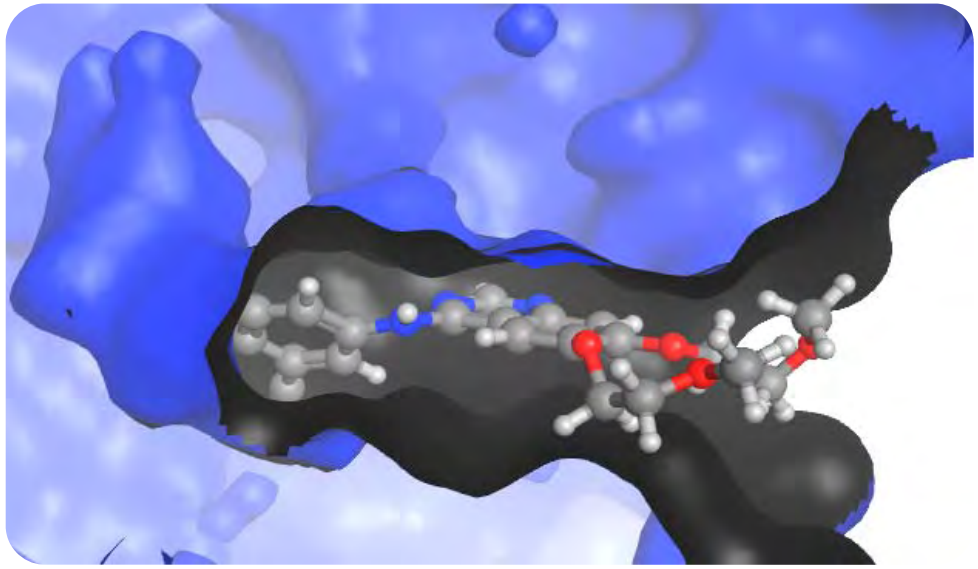
- Les implicacions de les conformacions en molècules orgàniques







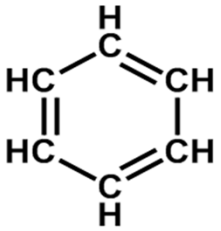


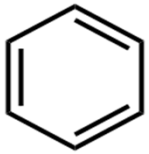


PDBID: 4HJO

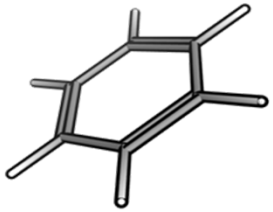
Representacions moleculars

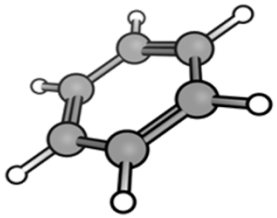
2D



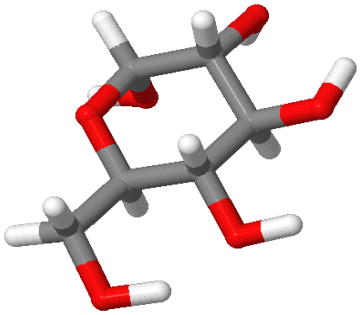


3D

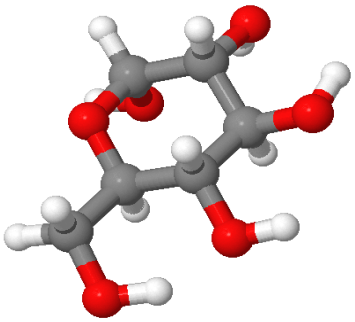




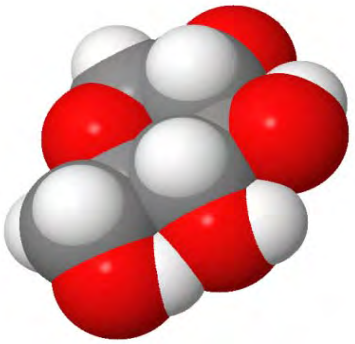
Jmol:



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

ZINC 12

Compound Search SM

UniProt

MolView AGPL Free Software Free as in Freedom

RCSB PDB
PROTEIN DATA BANK

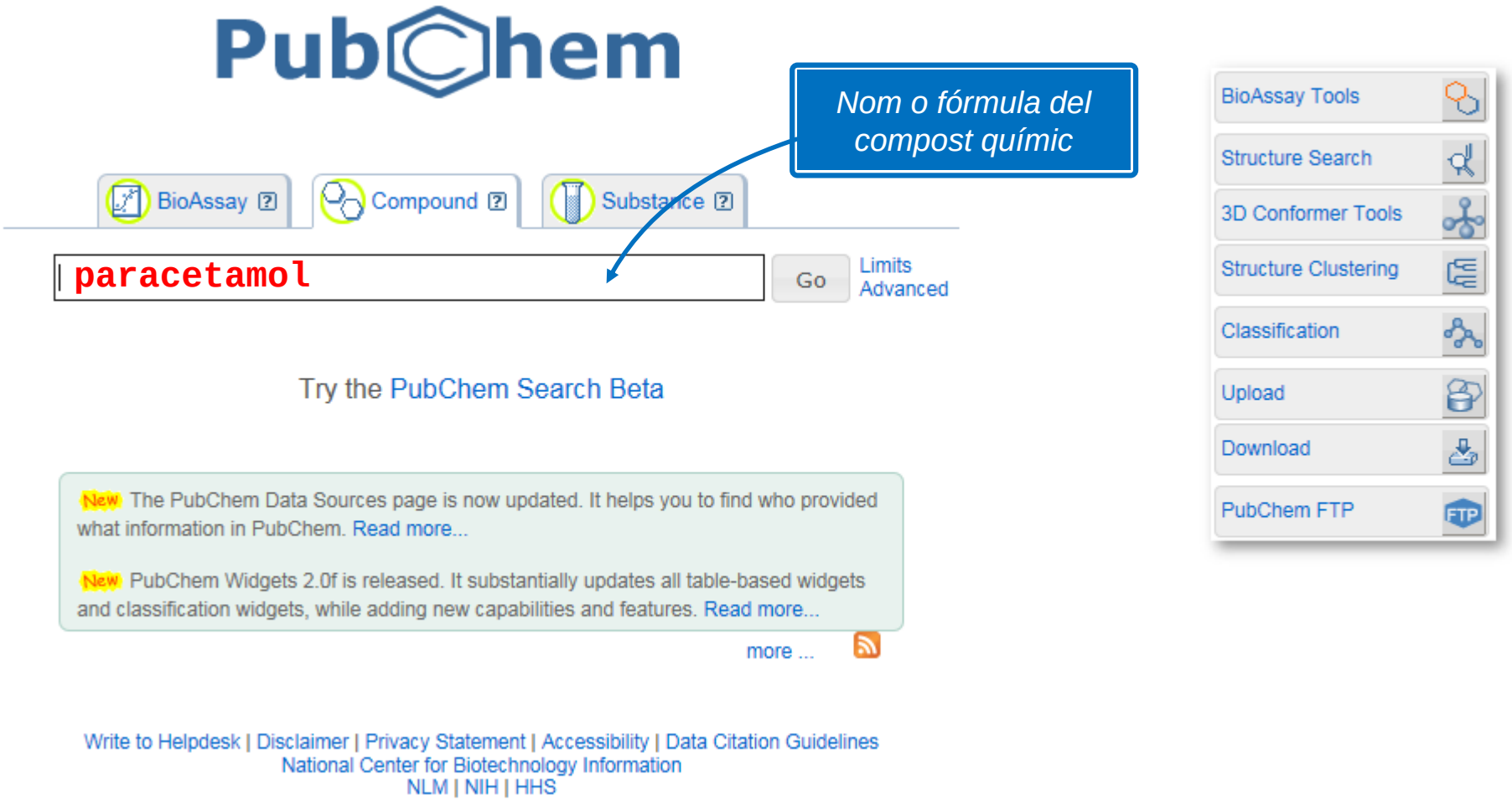
On podem trobar informació?

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

- 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,...

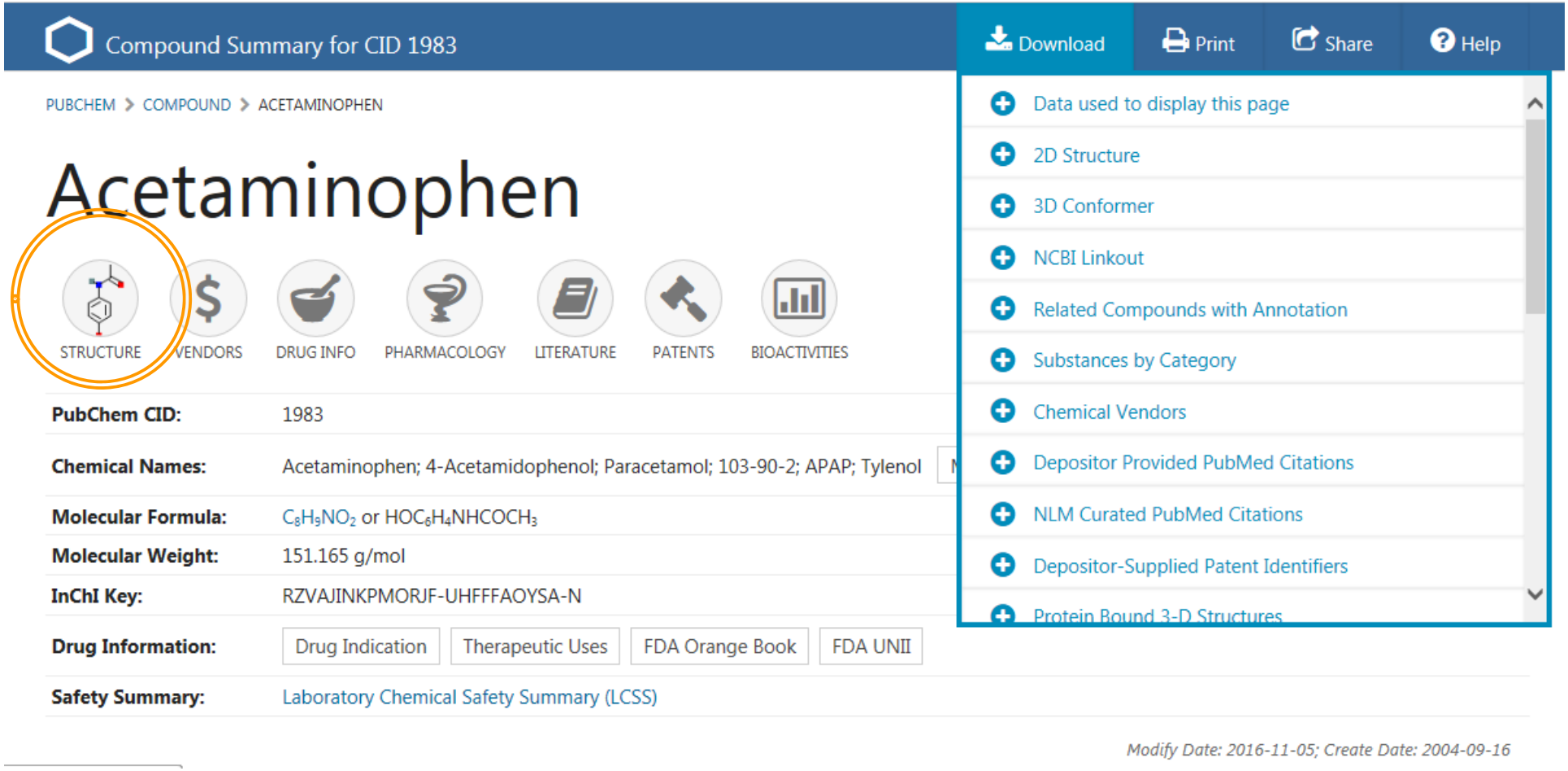
- Visualització d'estructures tridimensionals
- Fàcil interactivitat (conté un editor)
- Dades espectroscòpiques

PubChem



https://pubchem.ncbi.nlm.nih.gov/#

PubChem – Informació farmacològica

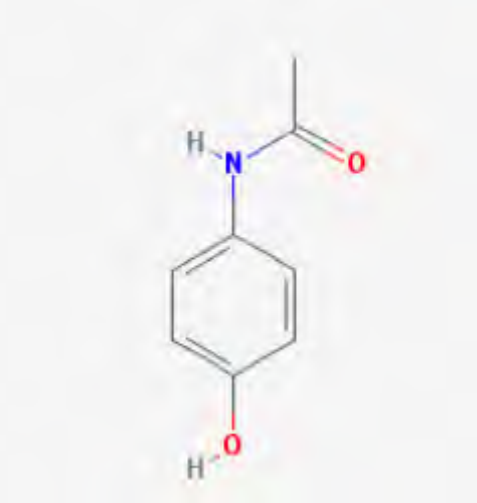


https://pubchem.ncbi.nlm.nih.gov/#

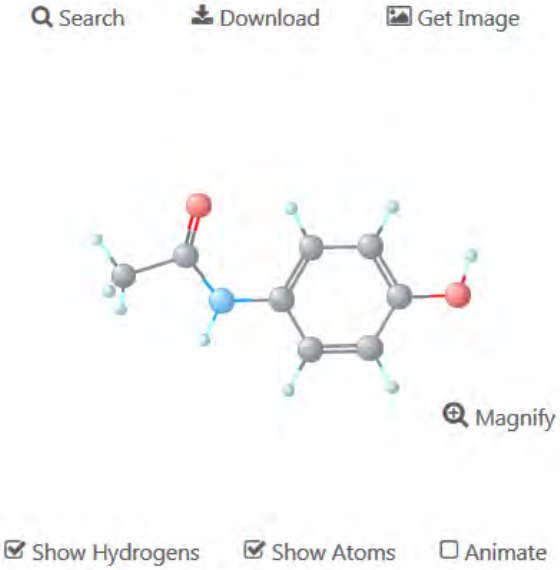
PubChem –Informació estructural

Contents

2D Structure



3D Conformer

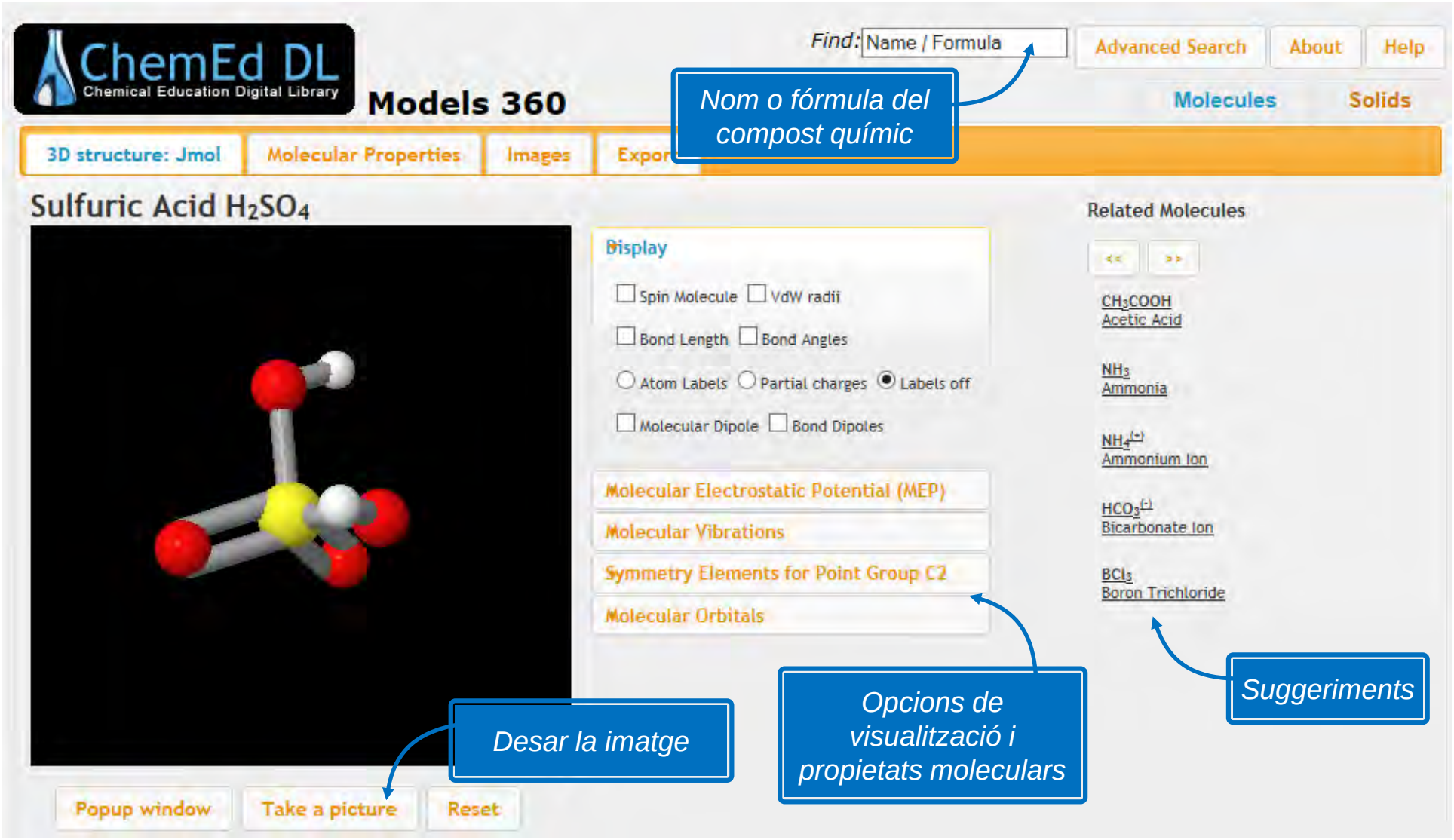


Names and Identifiers

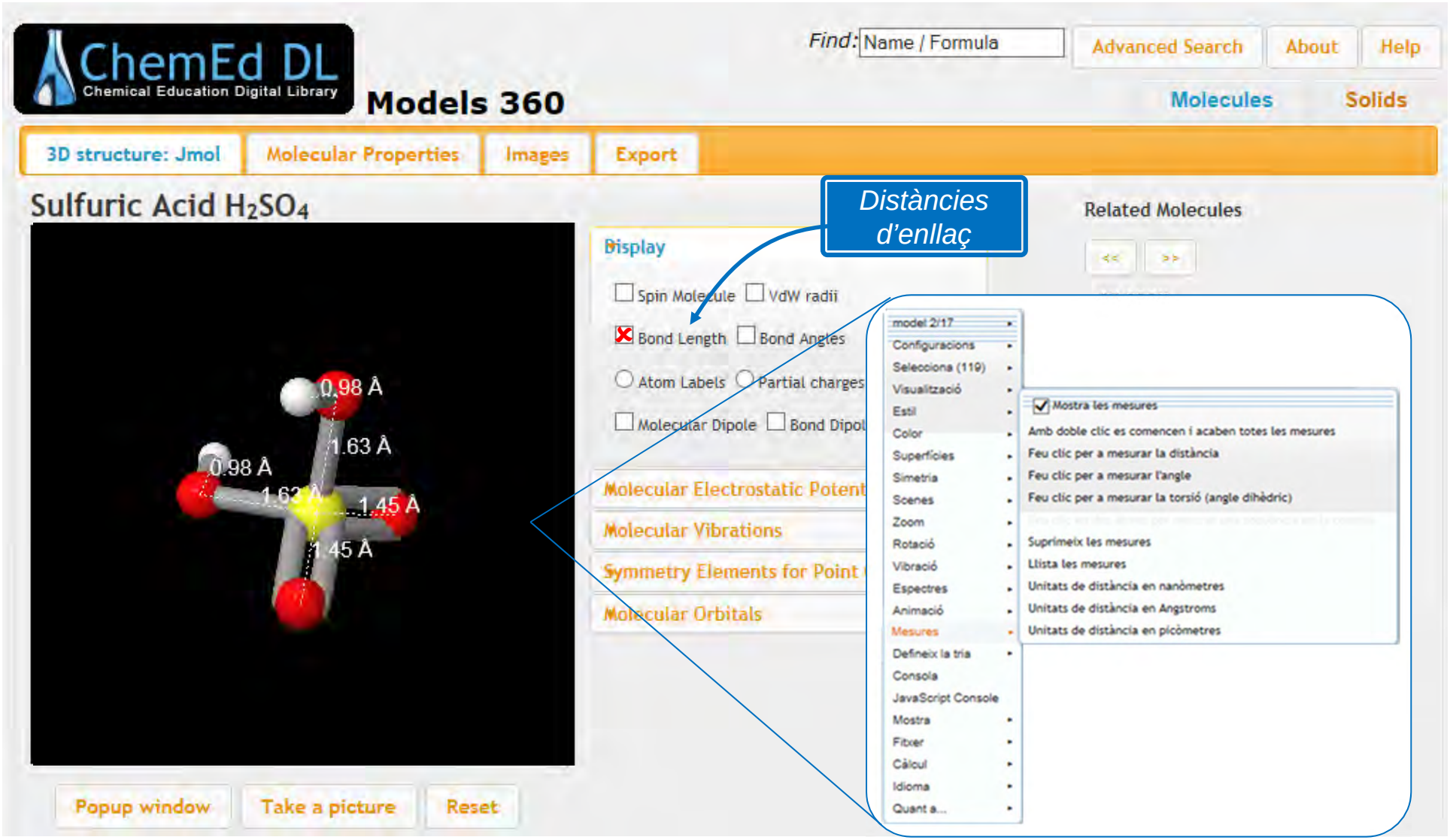
IUPAC: N-(4-hydroxyphenyl)acetamide
InChI Key: RZVAJINKPMORJF-UHFFFAOYSA-N
Canonical SMILES: CC(=O)NC1=CC=C(C=C1)O
Molecular Formula: $C_8H_9NO_2$

https://pubchem.ncbi.nlm.nih.gov/#

Models 360



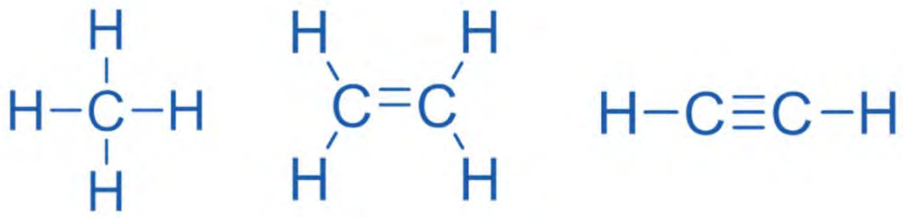
http://www.chemeddl.org/resources/models360/models.php



http://www.chemeddl.org/resources/models360/models.php

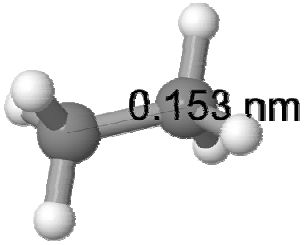
Per exemple...

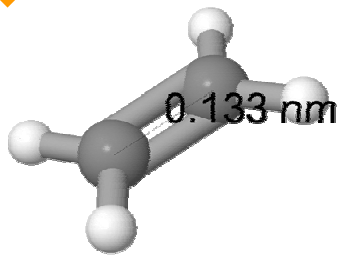
- Tots els enllaços C-C són iguals?

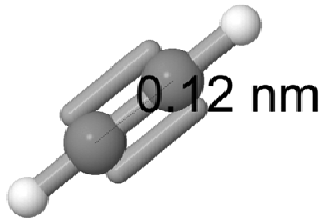


3D !

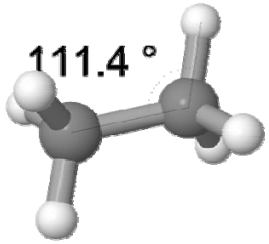
Distància C-C

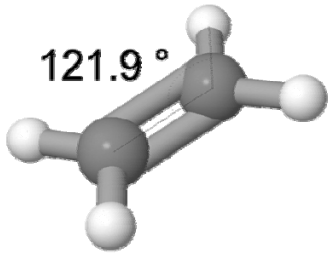


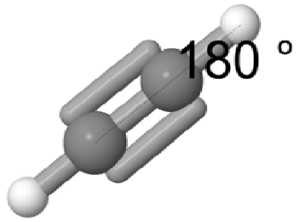




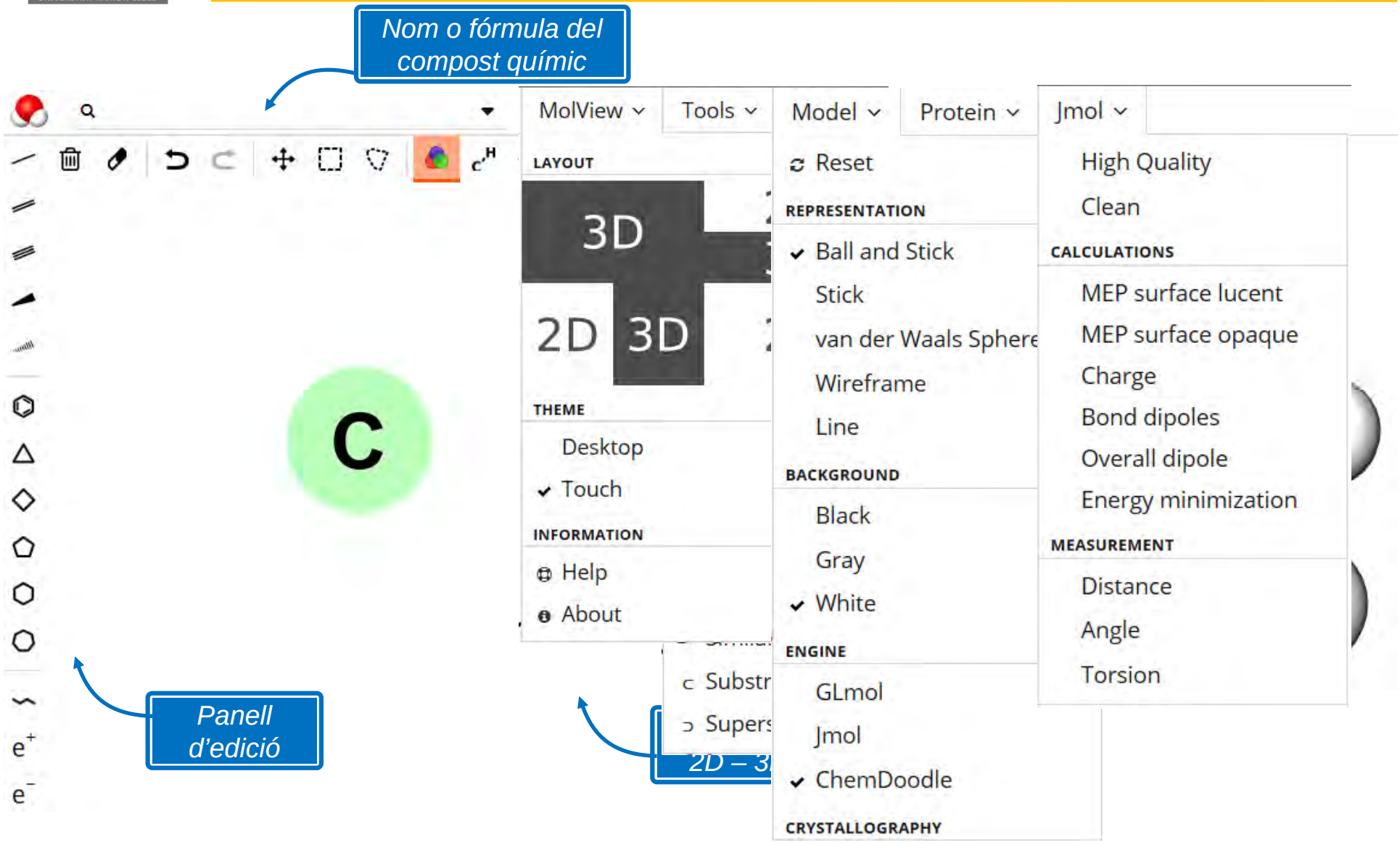
Angle H-C-C





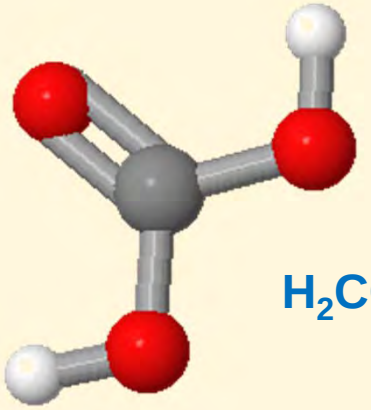


MolView

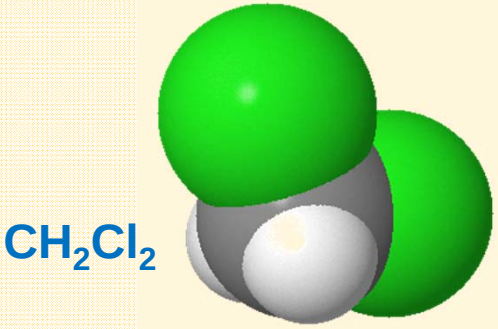

Nom o fórmula del compost químic
MolView
Tools
Model
Protein
Jmol
LAYOUT
3D
2D
3D
THEME
Desktop
Touch
INFORMATION
Help
About
Reset
REPRESENTATION
Ball and Stick
Stick
van der Waals Sphere
Wireframe
Line
BACKGROUND
Black
Gray
White
ENGINE
GLmol
Jmol
ChemDoodle
CRYSTALLOGRAPHY
High Quality
Clean
CALCULATIONS
MEP surface lucent
MEP surface opaque
Charge
Bond dipoles
Overall dipole
Energy minimization
MEASUREMENT
Distance
Angle
Torsion
C
Panell d'edició
2D – 3

Diferents tipus d'enllaç

Molècules enllaç covalent

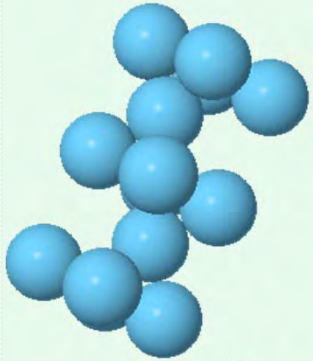


H_2CO_3

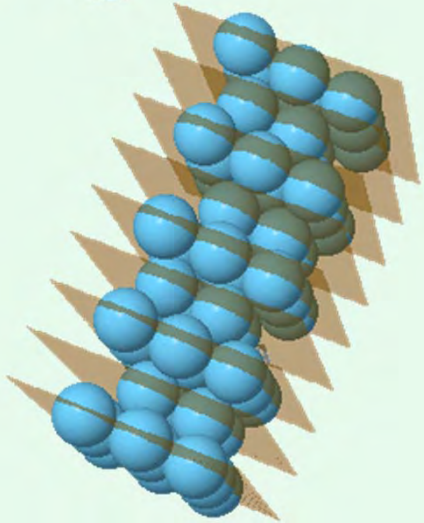


CH_2Cl_2

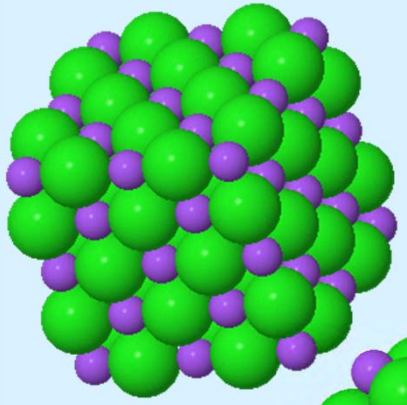
Estructures metàl·liques

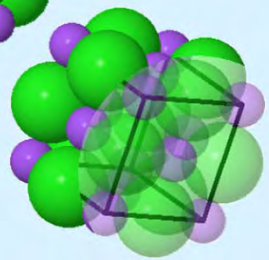


Ce

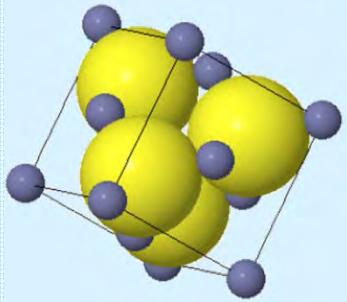


Estructures iòniques





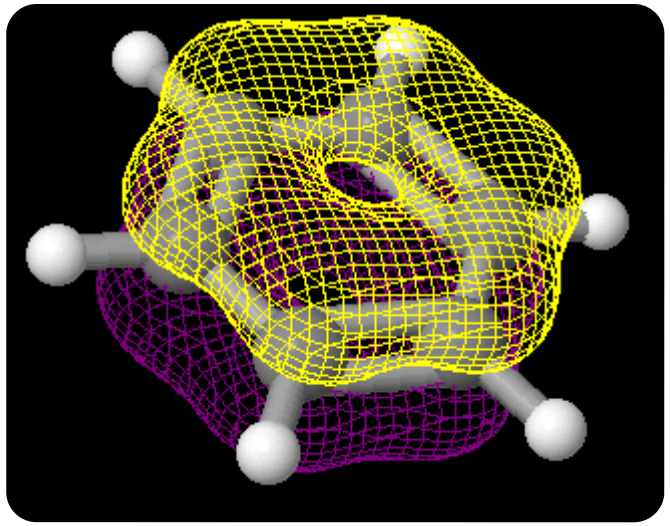
NaCl

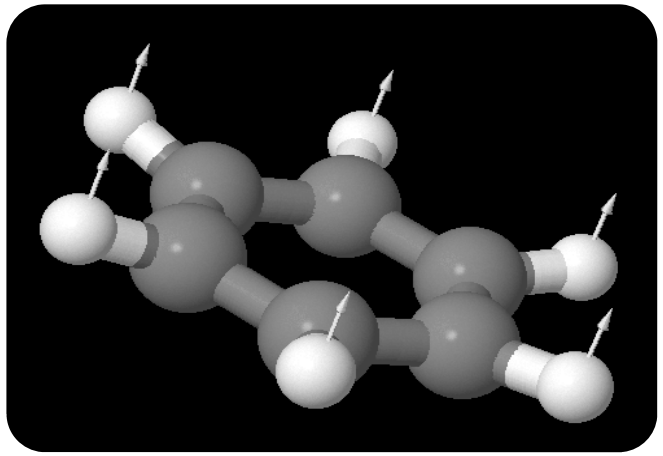


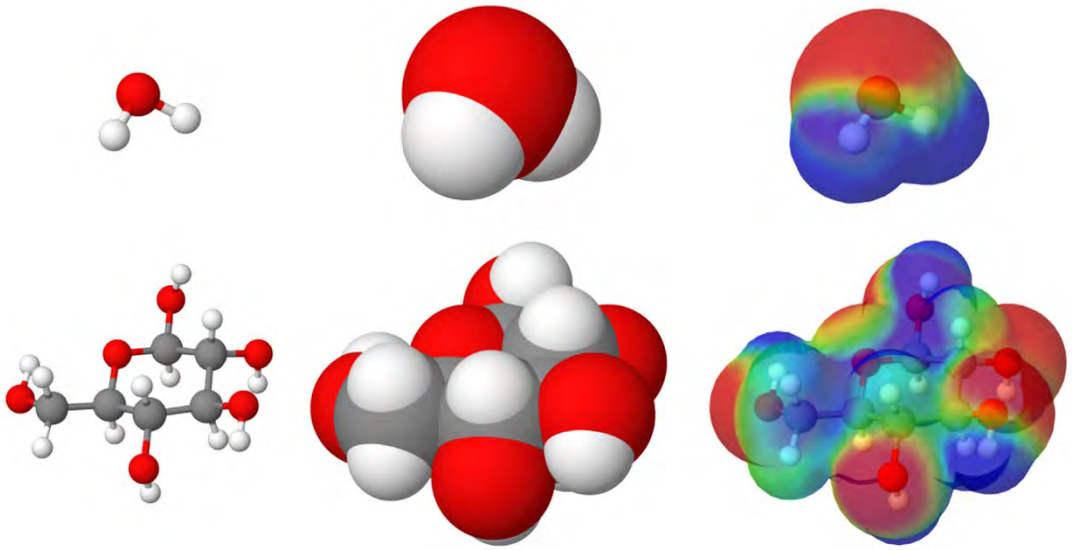
ZnS

Estudiant altres propietats

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

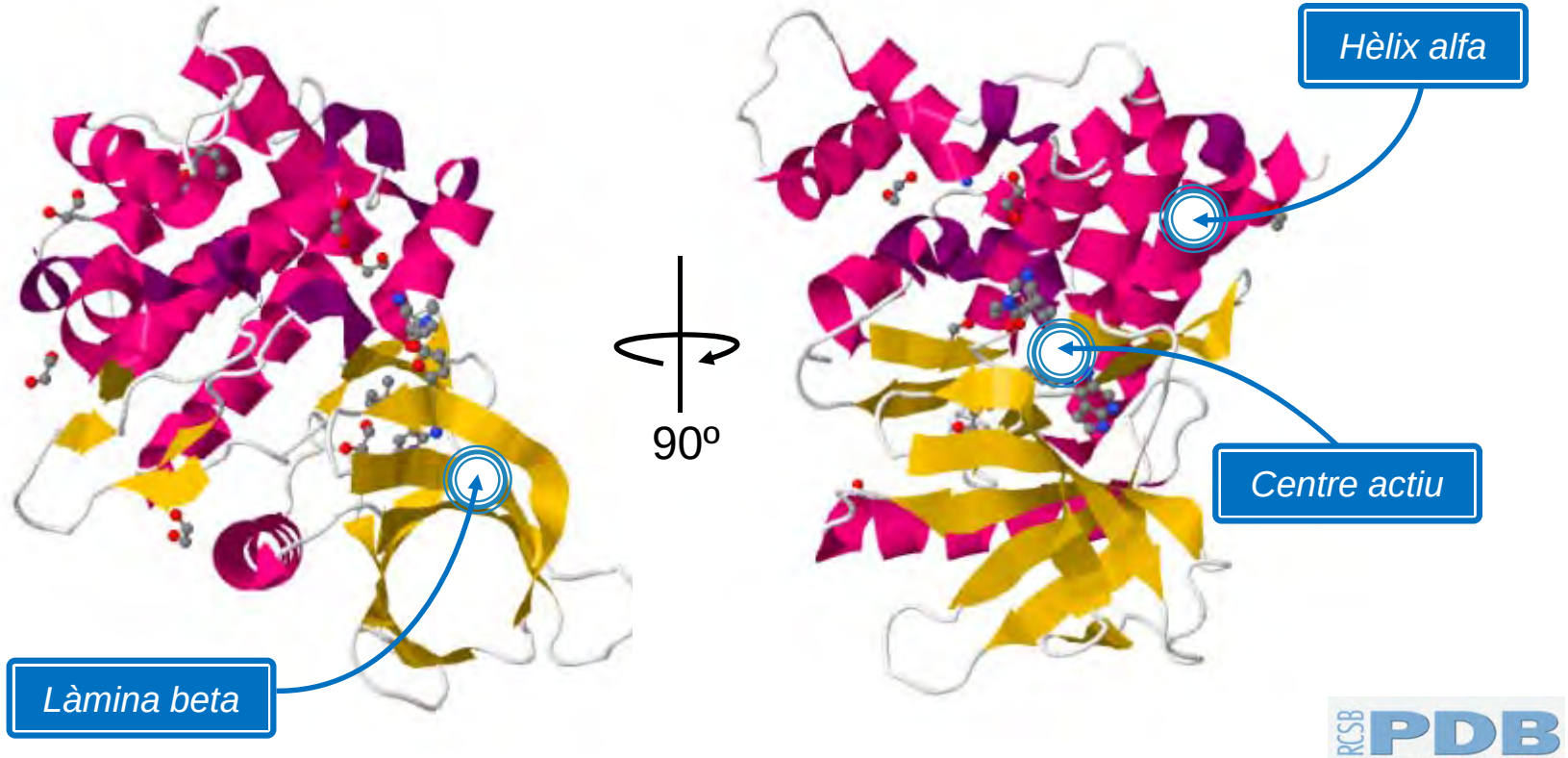






Sistemes biomoleculars

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



5LWN (http://www.rcsb.org/)

Del 2D al 3D

ChemSpider Search and share chemistry

ChEMBL

eMolecules

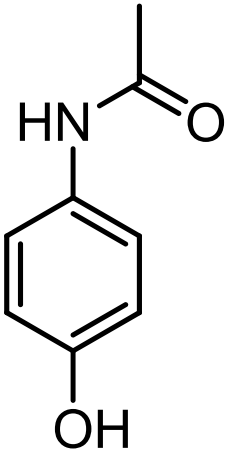
RCSB PDB PROTEIN DATA BANK

UniProt

DrugBank Drug & Drug Target Database

Compound Search

ZINC 12



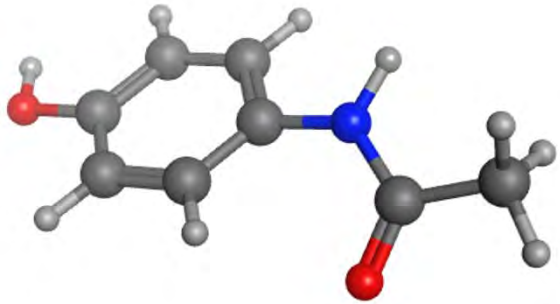
PubChem

MolView

AGPL Free Software Free as in Freedom

ChemEd DL Chemical Education Digital Library

Models 360



Moltes gràcies per la seva atenció!

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Agraïments: Dr. Jordi Cuadros, Dra. Laia Ros