

TEACHING CHEMISTRY WITH PORTABLE DEVICES

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Abstract

Chemistry is an abstract science in which a large amount of material has to be learned by the students. Using programs for visualization and calculation of properties, can help students to develop better skills in the learning of Chemistry.

In our course, at the Faculty of Chemistry (Universidad Nacional Autónoma de México, UNAM), we have implemented the use of iPad and iPhones for teaching Chemistry.

Several programs are used. With this tools, students improve their learning skill dramatically.

Keywords: Chemistry, Organic chemistry, Proteins, Reactions, Molecular modeling

1 INTRODUCTION

Chemistry is an experimental discipline, relies heavily in observation of exploratory results and the handling of data. A chemical structure is related with characteristic properties and their reactions. A name is given to a compound to characterize it, in many cases these names are trivial and one compound can have several names. In order to be more precise the chemists use the 2D graphical representation of chemical structure.

Several methods of shape recognition can be used to identify the structures, but variation in size and arrangement of the different part of a molecule can produce ambiguity.

The use of computers to teach chemistry is nowadays a common tool. The problem arises when a quiz has to be performed by the students, and the answers have to be evaluated by a computer. Graphic formulas can be handling very efficient with the computers.

1.1 Programs

Several programs can be used to handle different chemical concepts. We are using mainly 3 of them, they can be implemented in portable devices, and can communicate with servers to obtain information about computational calculations.

1.1.1 *iHyperchem*

This program allows the creation of molecules locally, along with their manipulation and display. The Level 1 version allows interaction with Professional HyperChem, Release 8.0.9 or later, over the internet. It allows sending molecules back and forth between the device and HyperChem as well as sending calculations to HyperChem via scripts and returning to log files.

For teaching how to build molecules and its shapes is a very useful tool. The communication involves the iPad or iPhone sending scripting commands to Professional Hyperchem. It acts as a Server to the portable device.

The basic idea normally involves manipulating a molecular system on the portable iPad or iPhone, sending it off to a Server to perform calculations on it and then returning a possible modified molecular system along with log file describing the calculation performed on the molecular system.

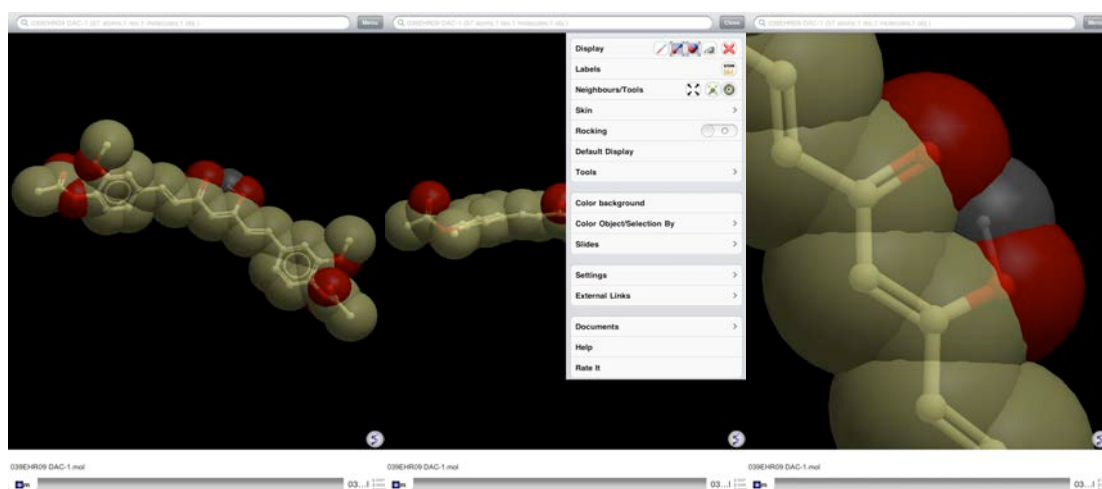


Fig1. Curcumin molecule in two representations

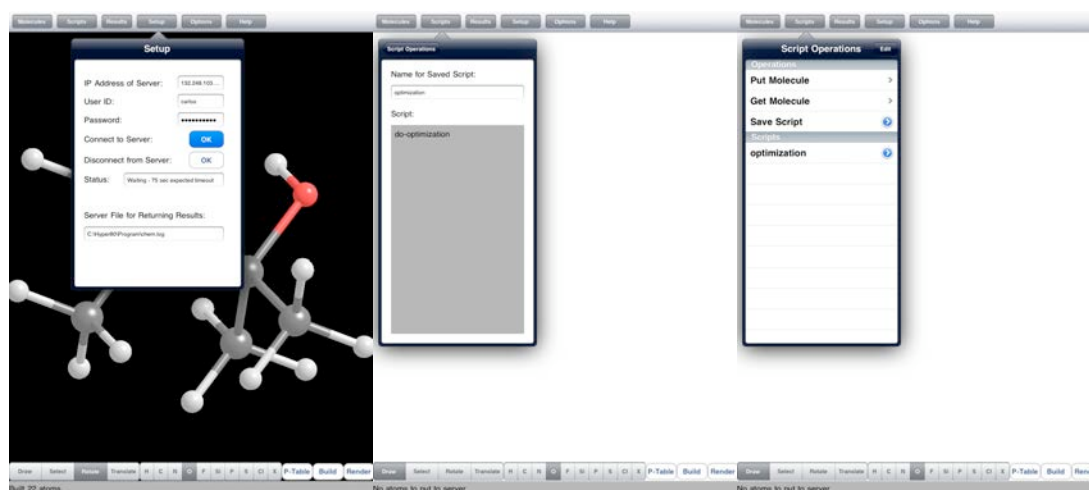


Fig 2. iHyperchem can communicate to a Server and proceed with Scripts to perform different tasks.

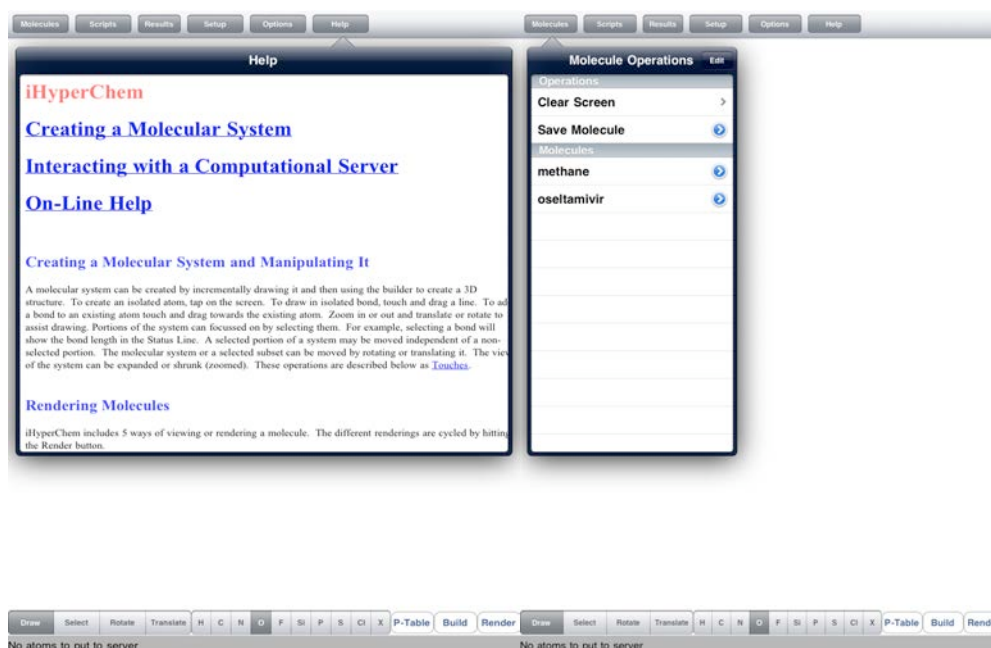


Fig 3. The program can create molecular systems and manipulating them, also the molecules can be saved for further retrieval.

1.1.2 iSpartan

Creates molecules as familiar 2D sketches, directly converts these into 3D structures, and calculates low energy conformations.

Atomic and molecular properties, NMR and infrared spectra, molecular orbitals and electrostatic potential maps are available from a 5,000 molecule subset of the Spartan Spectra and Properties Database (SSPD). The database may also be searched by substructure. Properties, spectra and graphical models of molecules in the SSPD subset are available for examination.

Several tasks can be done as: Conformational Analysis, finding properties, R/S chirality; LogP; Weight; Vicinal coupling constants; Area and Polar Surface Area; Measure distances, angles, and dihedral angles; Volume

A very important tool is the possibility of visualizing the NMR Spectra. With the assignment of proton and carbon NMR spectra; Confirm or challenge structure predictions based on NMR;

Suggest which structure best fits NMR data; Explore and suggest alternative structures

Thermochemistry; Identify best tautomer or isomer; Estimate equilibrium product distributions; Determine if reaction is endothermic or exothermic

Infrared Spectroscopy

Associate lines in an IR spectrum with functional groups; Confirm or challenge structure. Predictions based on IR; Animate molecular vibrations associated with peaks in spectrum

Molecular Orbitals and Electrostatic Potential Maps.

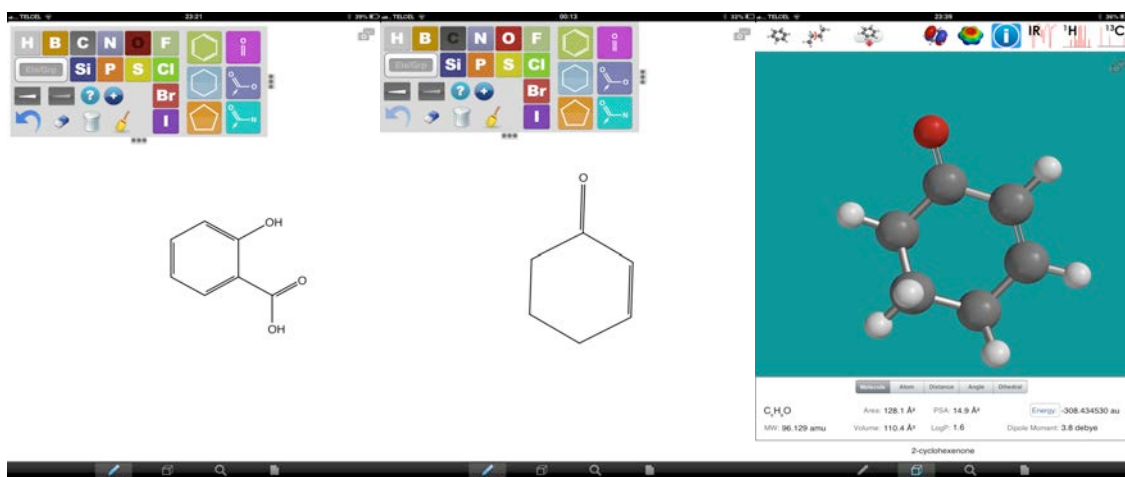


Fig 4. The tools for creating molecules are very easy to use. And different representations can be obtained.

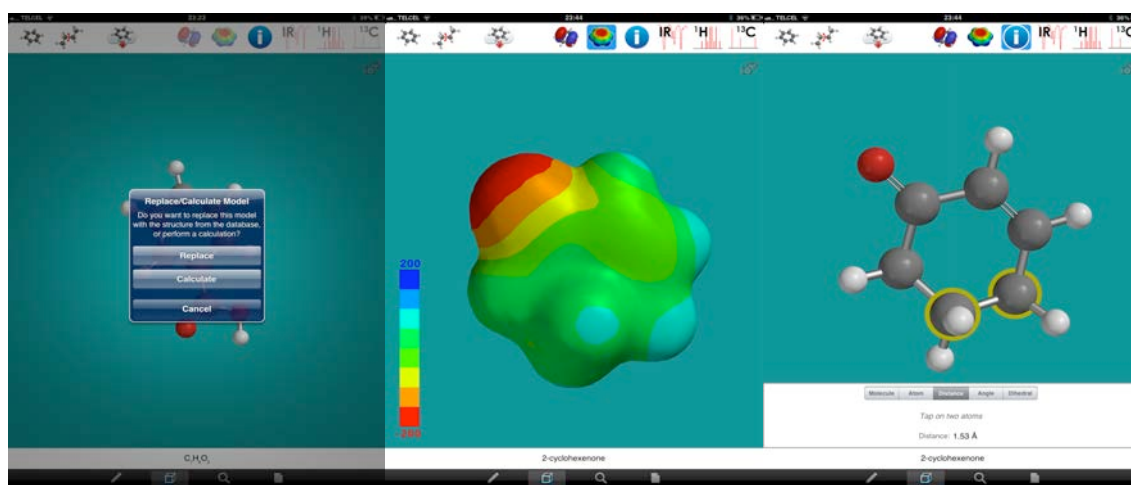


Fig 5. The molecules can be analyzed and obtain important information about the electronic configuration and the geometry of the molecule.

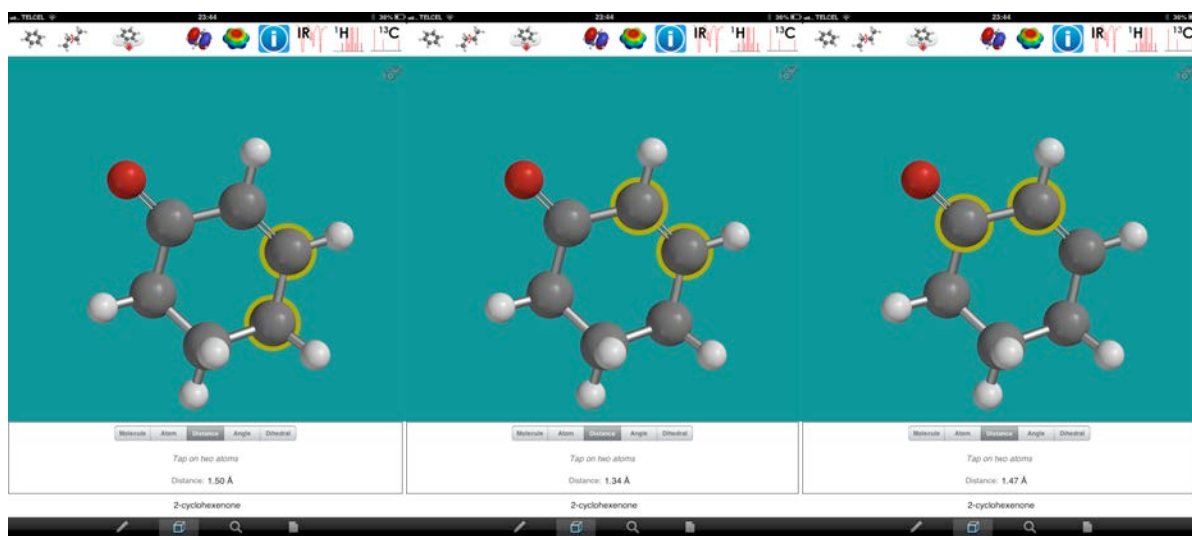


Fig 6. The distance of different type of bond can be analyzed in a visual and interactive way.

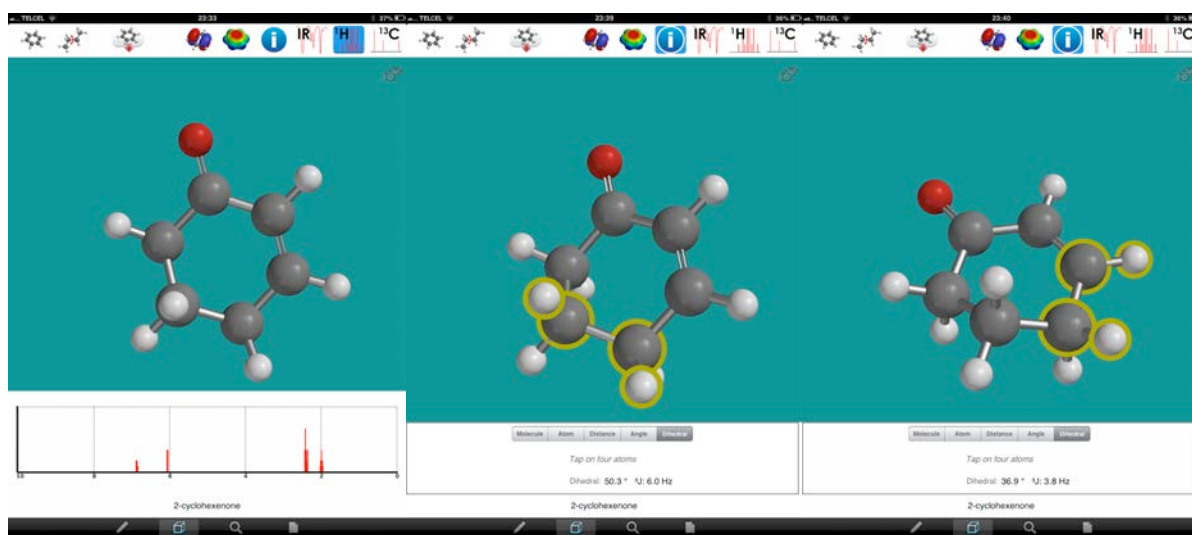


Fig 7. The simulation of the NMR spectra are very useful for the interpretation of the structure, also the coupling constant of the vicinal hydrogen can be calculated.

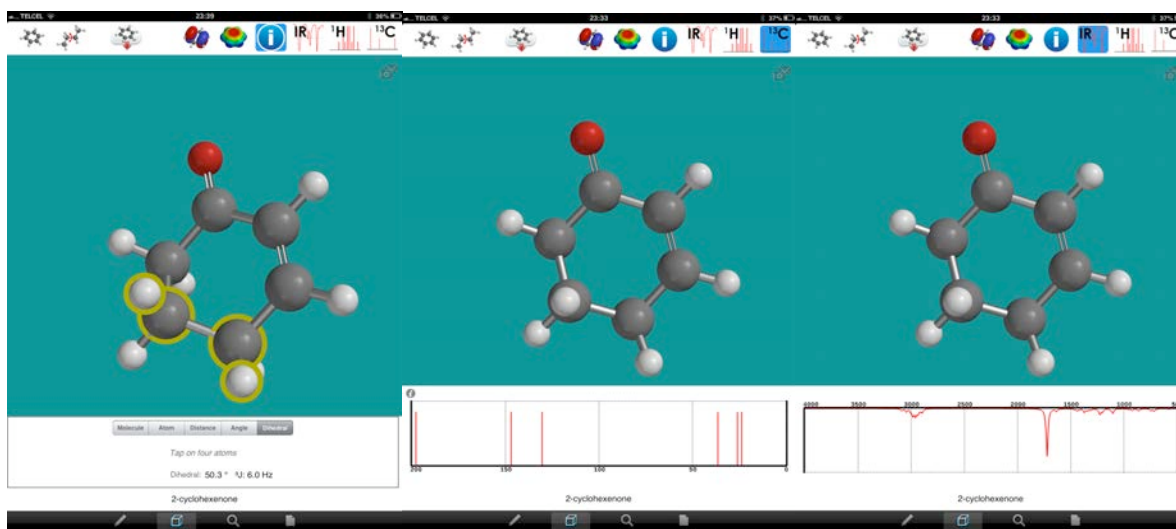


Fig8. The NMR of the C13 can be simulated, and also the IR vibrations of the molecule.

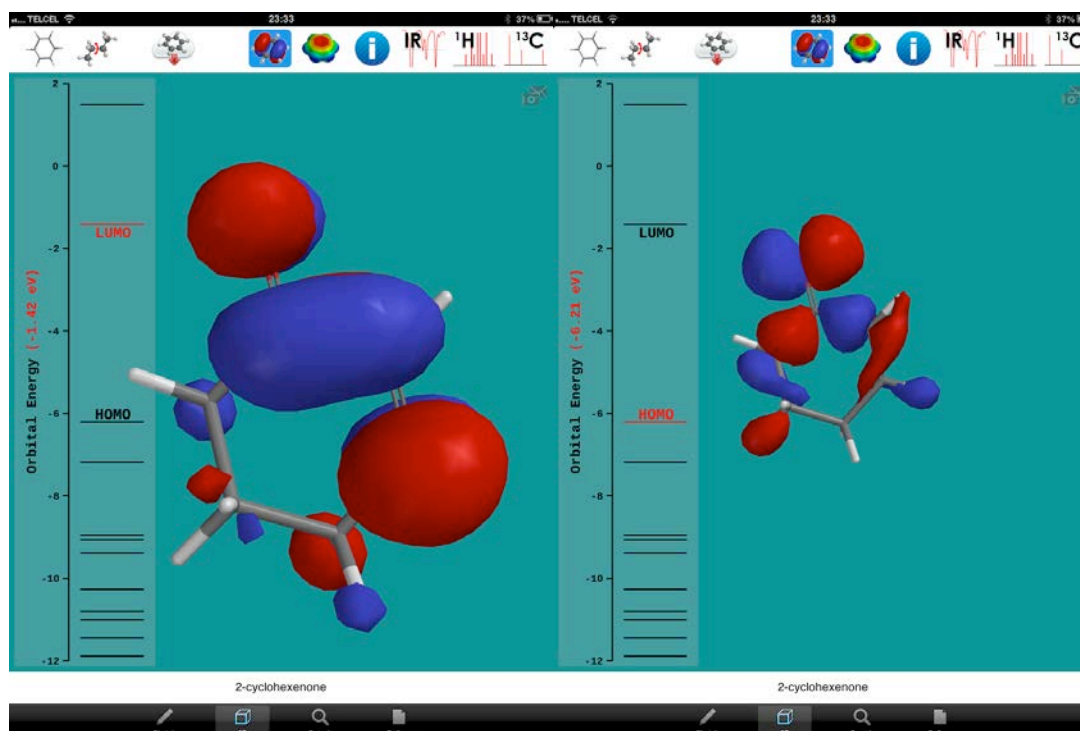


Fig 9. The calculation and visualization of the orbitals, HOMO and LUMO can give very important information about the reactivity of the molecules.

1.1.3 iMolview

It allows the search for drugs in DrugBank, or proteins in the PDB and immediately explores their structure and annotation. This program is more useful for large molecules.

The key features present in the program are:

- Save structure and slides (molecular document).
- A direct link to the Protein Data Bank (PDB) and DrugBank.
- Superimpose multiple objects
- Side by side stereo
- Angle and distance measurement
- Each molecular view can be customized with a rich set of molecular representations including:
 - wires, balls-and-sticks, space filling, ribbon diagrams, and molecular surfaces.
- Zoom in and out, rotate, spin, pan, and clip the 3D molecule.
- Search and download structures from NCBI website.
- Read in any PDB file from any URL.
- A wide selection of coloring schemes is available.
- Color background, color molecule by atom type, chain, N- to C- terminal, and secondary structure.
- Select residues, atoms, or chains and color or change their representations individually.
- Select residues in sequence and get the corresponding selection in 3D.
- Select the whole chain by holding the corresponding tab.
- Display Fog Effect
- Saving Slides and Documents
- Slide is a combination of a view point and graphics representation. In iMolview you can create multiple slides and access them later after the document was saved.
- To create a slide:

- Setup a view and representations (color, label, etc.)
- Go to Menu/Slides and choose "Save Current View"
- Give a name and press 'OK'. It should appear in the list
- Repeat these steps to create more slides

Supported file types are:

- ICB: Molsoft molecular document format. May contains multiple molecular objects, meshes slides and others.
- PDB: Protein Data Bank file.
- MOL/MOL2: MDL or Tripos small molecule file.
- PARAM can be one the following:
- BGCOLOR: redefine the background color. The VALUE should be a color name.
- PDBCODE: loads PDB structure with the code from VALUE. If you have this field PATH_TO_THE_FILE should be omitted.
- SLIDE: sets the slide. The VALUE should be either slide name or number
- RUN: runs a list of semicolon (or new line) separated lits of ICM script commands.

Examples:

```
# opens the document and sets the default view.
imolview://History/3gvu.icb
# opens slide 1
imolview://History/3gvu.icb?SLIDE=1
# opens slide 'Slide2'
imolview://History/3gvu.icb?SLIDE=Slide2
# opens default view for PDB '1xbb' sets background color to white
imolview://?PDBCODE=1xbb&BGCOLOR=white
# loads PDB and highlights the ligand
imolview://?PDBCODE=1xbb&BGCOLOR=white&RUN=display a_A,N ribbon transparent;color
ribbon rgb={200,200,200}; display cpk xstick a_H; center a_H
```

The different versions have introduced more features:

Version 1.6

- Added interface to Dropbox (Documents/Dropbox)
- Added molecular skin/surface representation
- Added "Tools/Filter Selection" to adjust the current selection by various parameters
- "Color Selection" can color individual representations.
- ICM scripts embedded with the ICB file are available in the menu.
- Added full screen mode.
- Added interface to the ICM command language (Command tab in the search bar)
- Tools menu (sbs stereo, measurements) appears for small molecules
- 2D labels are displayed properly

Version 1.5

- Major:
- retina (high res) display support for the new iPad
- multiple object support + superimpose
- Others:
- assign secondary structure

- images in html pane
- side-by-side stereo
- angle and distance measurement
- email screen shot

Version 1.4

- added auto 'rocking&rotation mode'.
- custom URL scheme imolview:// is extended to allow open document on the particular slide (from the webpager, keynote or other apps)
- Added the ability to save molecular document (structure + slides).
- Added the ability to save view and representation (slides).
- Fixed memory leak in xstick display
- Fixed crash in 3D labels

Version 1.3

- support for horizontal screen orientation
- support for custom URL scheme (imolview://)
- search results are now scrollable and load more hits
- VGA output on iPad and iPhone4 (3D view is mirrored, 'laser pointer' appears on touch and hold)
- improved selection in sequence view (residue range is shown). Fixed bug with selecting single residue.
- added atom labels display
- added centering without zoom (via center button in menu)
- preferences are now persistent even if the app is closed and opened again
- added preference for hydrogen display (none/polar/all)
- added default url preference for loading molecules off a web page

Version 1.2

- issue with older iPhone/iPod devices FIXED
- structure files (pdb/icb) sync via iTunes
- download history
- easy toggle of individual molecule display via sequence view tabs
- faster refresh in CPK representation
- display tools popup bar on selection
- improved handling of very large structures
- neighbors in other chains selection, such as atoms in the vicinity of selected ligand
- external links menu: Uniprot and RCSB entries in addition to PubMed
- atom type coloring for hetero-atoms only - allows combining chain-specific colors and atom type color coding
- 3D residue picking is now tracked in sequence view
- easy clear display button (X)
- bug/crashes fixes

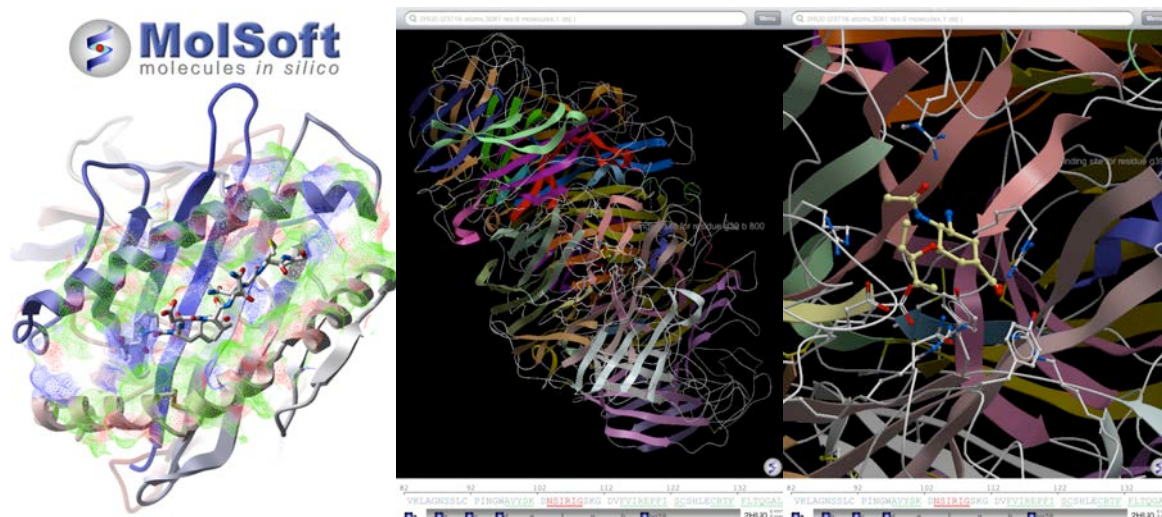


Fig 10. Large molecules of proteins can be studied and visualized in different representations.

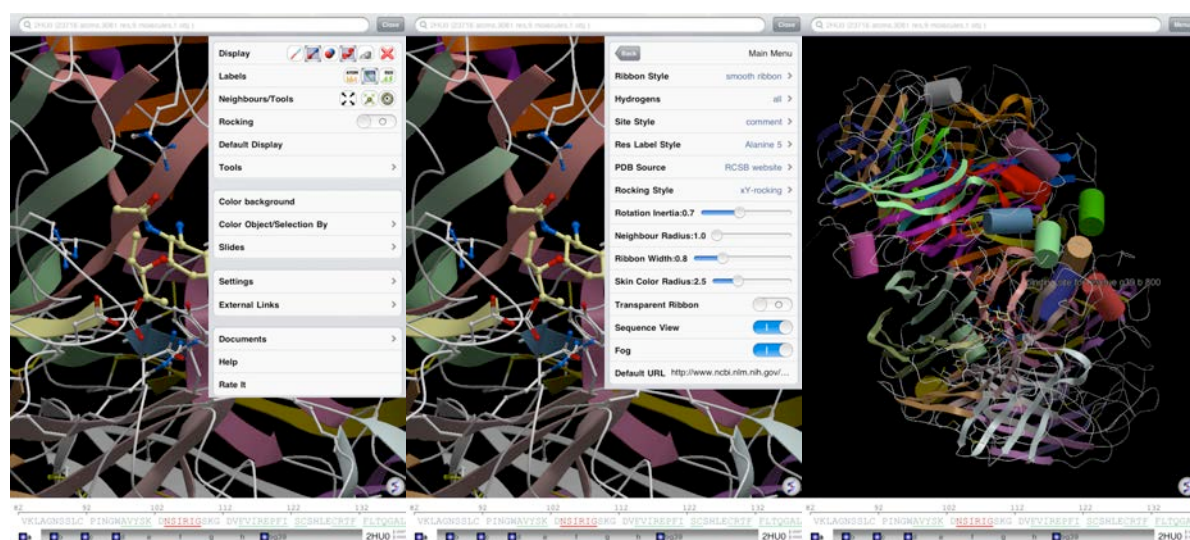


Fig 11. The drop menu is very useful for changing parameters.

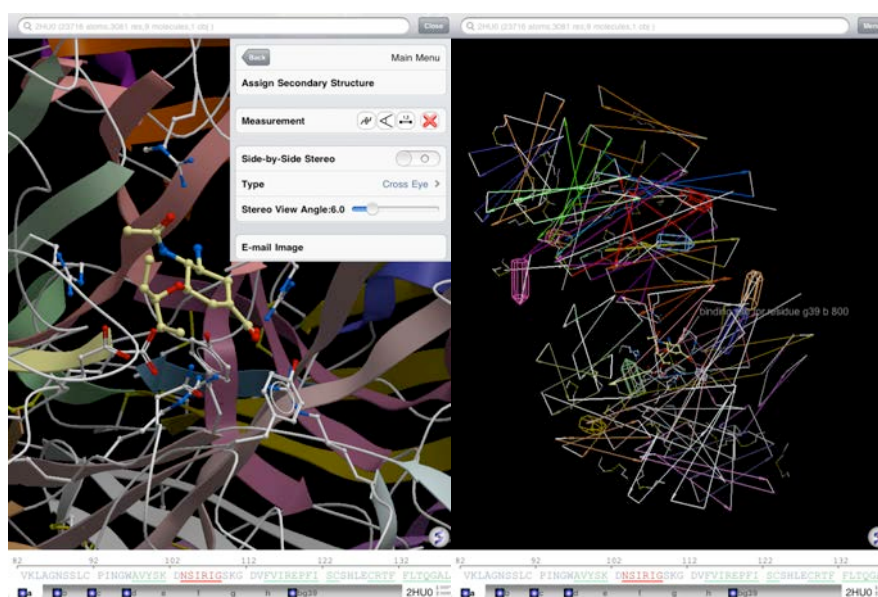


Fig 12. The large variety of representations and the calculations that can perform make it a very valuable tool for understanding biomolecules.

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