# MolSoft's Latest News

MolSoft

January 2011

Dear ICMers,

Happy New Year!

Welcome to MolSoft's latest newsletter which includes information on a new ICM Force Field, ICM on the iPhone and iPad, the upcoming ICM Scripting Workshop, and the location of MolSoft's new office in San Diego and other news… We also include some answers to some recently asked questions about ICM. You can also follow MolSoft on Twitter, Facebook and Youtube.

NEW ICM VERSION 3.7 RELEASED!

Please download the latest version (v.3.7-2) of ICM from our support site. The new features are listed here along with some screenshots. Some of the new features include:

- New ICM force field.
- New easy to use HTML editor for creating molecular documents.
- WebKit integration into ICM.
- Charge protonation state prediction using a pKa model.
- Explicit group docking.
- Implicit membrane models.
- And much more…
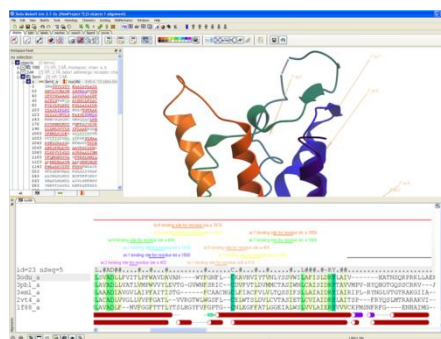
NEW ICM FORCE FIELD

Scientists at MolSoft have developed a new physics-based internal coordinate mechanics force field. Please see the publication in the Proteins journal by Arnautova *et al* (Proteins 2010) where the force-field has been applied to protein loop modeling. The new force-field contains new parameterization for the dielectric constant, an improved hydrogen bond determination method, and implementation of novel backbone atom torsional potentials which include bond angles of the carbon (alpha) atoms into the internal variable set.

Follow these instructions to use the new force-field in your own scripts for energy minimization or optimization. If you want to use the force field for loop modeling please use the

_loopmodel macro where the following parameters are preset.

1. Use the latest ICM version 3.7-2a which can be downloaded here.

A set of loop conformations generated in ICM using _loopmodel macro.

2. The polypeptide must be built or converted with the icmff residue library to do this:

LIBRARY.res = "icmff"

read library

3. The dielectric constant should be set to 2.

dielConst = 2.

4. In addition to regular energy terms, "bb" must be turned on

set term "bb"

5. The force-field method should be set to icmff

ffMethod = 4

UPCOMING ICM SCRIPTING WORKSHOP

February 3-4 2011 – San Diego, CA
We will be holding a 2-day ICM Scripting Language workshop on Feb 3rd-4th 2011. This workshop will teach you from first principles all you need to know about ICM scripting so you can automate your work using ICM and write your own macros and scripts. This workshop is relevant to all ICM users and no previous knowledge of ICM scripting is required. More information here:

You will learn:

- The basics of the ICM Scripting Language
- Advanced data types and operations
- Molecules, sequences and meshes
- Working with Macros and scripts
- Graphical User Interface Programming in ICM
- Input/Output and External Services
- ActiveICM and Web Publishing

The workshop will be conducted by:
Ruben Abagyan Ph.D. (Professor, UCSD)
Max Totrov Ph.D (Principal Scientist, MolSoft LLC)
Eugene Raush, M.Sc. (Principal Developer, MolSoft LLC)

NEW FEATURES ADDED TO FREE ICM-BROWSER - DISPLAY FULLY INTERACTIVE MOLECULES IN POWERPOINT AND THE WEB

In case you did not hear we have added many new features to our free ICM-Browser product. These new features include:

Build and save fully-annotated and interactive 3D molecules and display them in Safari, Firefox, Google Chrome, and Internet Explorer.

- Display fully interactive molecules in Windows PowerPoint.
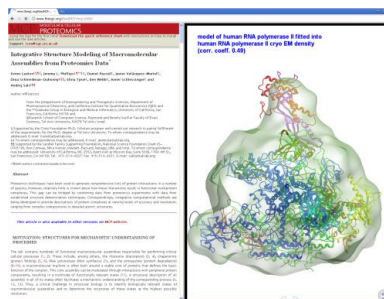
- Display ligand pocket surfaces colored by binding property.
- Add and optimize hydrogens to a PDB structure.
- Calculate and display hydrogen bonds.
- Generate and display molecule surfaces.
- Display transparent surfaces.
- Save publication quality molecular graphics files in a variety of image formats.

It is easy to get started:
1. Click here to download the ICM-Browser software and click here to download the ActiveICM plugin.

2. Follow the links to the documentation and help videos here.

MOLSOFT HAS MOVED TO NEW CUSTOM BUILT OFFICE LOCATION

After more than 10 years in La Jolla, MolSoft has now moved to larger custom designed offices in Sorrento Valley. Our new address is: 11199 Sorrento Valley Road, S.209, San Diego CA 92121 – not very far from our previous location.

See a map here. All our phone and fax numbers remain the same.

NEW ICM HELP VIDEOS ON YOUTUBE

We have placed a number of new help videos on our Youtube site. The recent ones cover many of the new ICM-Browser features. Click here to view the site.

CONGRATULATIONS TO OUR COLLABORATORS AT THE SGC FOR SOLVING THEIR 1000TH CRYSTAL STRUCTURE

The Structural Genomics Consortium (SGC) solved their 1000th crystal structure in 2010. The SGC press release has some very nice ICM generated graphics!

RECENT FAQS

What do the options in Docking/Preferences/Charge Groups mean? This relates only to the ligands:

- NH2 = ICM will charge primary amines only
- NH2 NH = ICM will charge primary & secondary amines only
- NH2 NH NT = ICM will charge primary & secondary & tertiary amines only
- NH2 NH NT = imidazole ICM will charge primary/sec/tert and imidazoles.

In the very latest version of ICM we have a prediction of pKA which will automatically charge each ligand according to the pKA prediction.

If you want to change the charge of the residues on the receptor please right click on the

ligand select mutate and there are uncharged versions of each residue available to select. If you do this then you would have to re-make the maps.

How do I sample macrocyles in ICM docking? MolSoft's ICM docking algorithm has flexible ring sampling included on the fly. Just set ring sampling level to 1 (flex ring only in pre-sampling step) or 2
(throughout the simulation). To do this:

- Set up the docking project.
- Before running the docking simulation go to Docking/Preferences/General and change the flexible ring sampling level to 1 or 2.
- Now run the docking simulation.

Or, If you want to generate the conformations before docking a then you can use the conformation generator algorithm described here.

How do I change the working directory? This is a common question from people who use ICM in Windows for small molecule and protein-protein docking. By default all the docking files are stored in a directory in "My Documents". This may not be convenient and so the way to change this is to use the command line and type:

set directory "c:/path_to_directory/"'

In the very latest version of the software there is now a GUI button to do this in the Tools menu.

How do I remove unwanted metal and counterions from an SDF file? You can do this in the menu option Chemistry/Standardize and check the remove salt option.

Can I make a selection by typing in the residue numbers? Yes you can. This is a common question primarily because this option is very well hidden! It is hidden for a reason because the residue numbers you enter can only relate to one molecule in a particular object. Therefore to find this option you need to right click on the molecule name in the ICM Workspace and choose Select/by Res.Number. You can then enter the residue numbers e.g. 3,7:12,30 and the selection will be made. If you want to make a selection on multiple molecules you can change the selection mode to add and repeat the steps described above.

How to Undertake Explicit Group Docking. In the very latest version of ICM you can define certain residues to be explicit during grid docking. For example, the hydroxyls of Ser, Thr, and Tyr can be treated explicitly during docking. We have written a tutorial on how to use this new docking option.

How to use the new HTML Editor. A new HTML WYSIWYG editor is now available that provides an interface which resembles how the page will be displayed in a web browser - no knowledge of HTML is required! You can also insert checkboxes, tables, images, external links, and ICM scripts into your HTML page. Please see the graphical user interface manual here for more information.

ICM ON THE IPHONE AND IPAD – COMING SOON!

ICM will soon be released on the iPhone and iPad where you will be able to use the app to browse PDB structures and sequences. We will let you know as soon as it is available for download but in the meantime here are some screenshots.
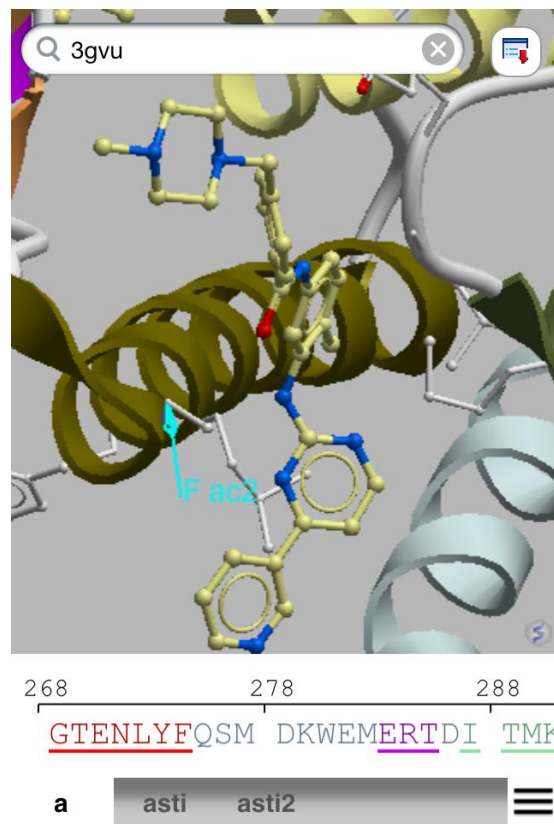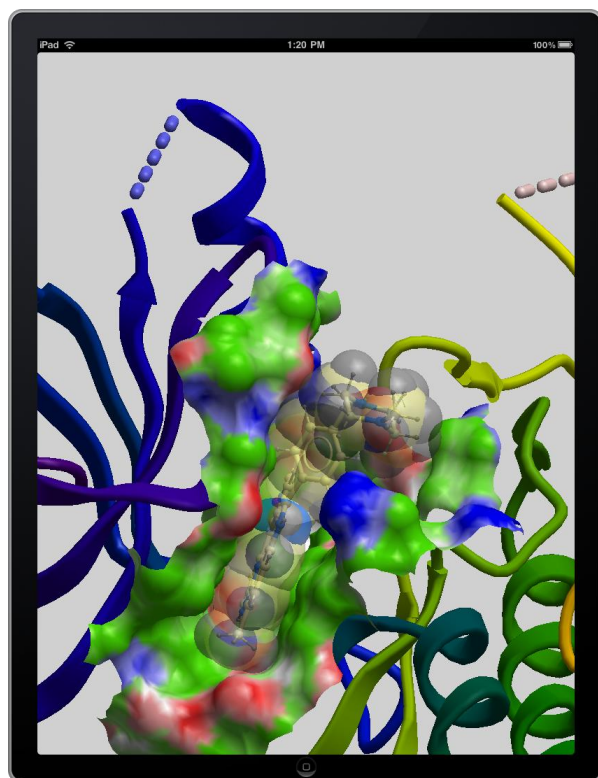
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