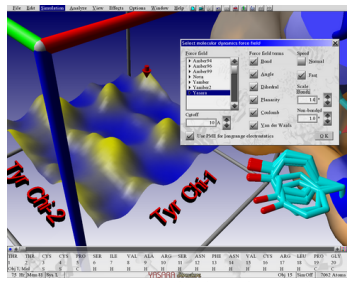
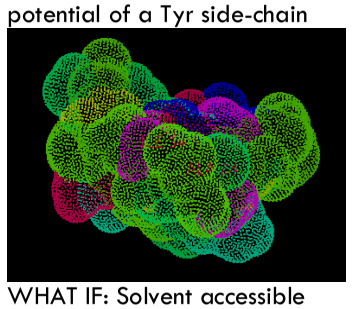
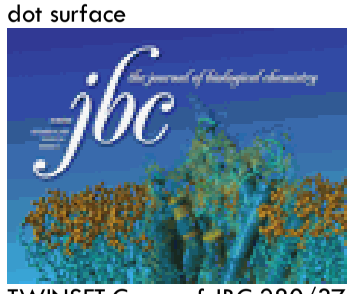
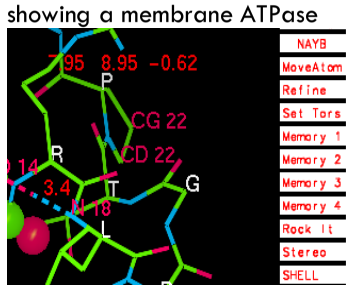


TWINSET: Knowledge based potential of a Tyr side-chain

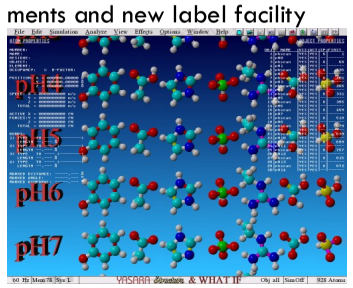

WHAT IF: Solvent accessible dot surface



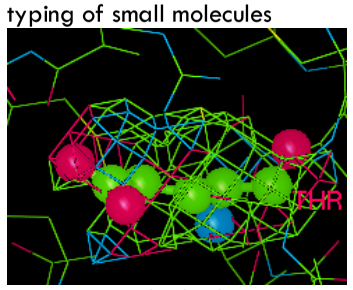
TWINSET:Cover of JBC 280/37 showing a membrane ATPase

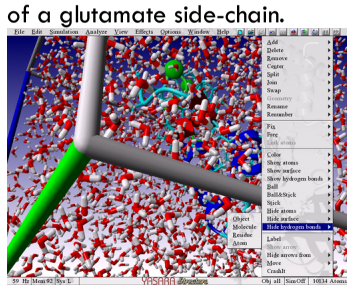


WHAT IF: Distance measure-ments and new label facility



TWINSET: pH dependent typing of small molecules


WHAT IF: Multiple density maps of a glutamate side-chain.


TWINSET: Real-time molecular dynamics simulation

Twinset highlights

The Twinset unites WHAT IF and YASARA behind a convenient user interface, including unlimited undo/redo. From YASARA, the Twinset inherits the following highlights:

- Photorealistic real-time (OpenGL) and publication quality (ray-tracing) graphics to illustrate your favorite journal cover or create molecular animations and encode them as MPEG movies.
- A human-readable selection language:

```
ShowAtom all with distance<5 from residue ATP
ColorRes Arg with contribution to molecular surface of object
 1crn, yellow
```

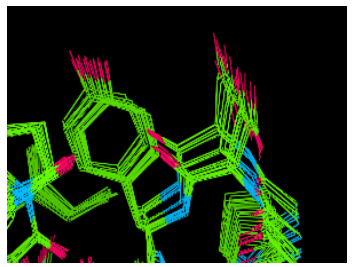
- Support for over 70 molecular file-formats.
- Automatic typing of small molecules, assignment of fractional bond orders and pH-dependent protonation: www.yasara.org/typing
- Semi-empirical quantum chemistry to optimize small molecules.
- Molecular simulations on a laptop at the speed of a cluster, using AMBER and newly developed force fields (NOVA,YAMBER).

  (E. Krieger et al., Proteins (2002) **47**,393-402 and Proteins (2004) **57**,678-683).
- Interactive simulations, pull atoms or entire molecules around and work with dynamic models instead of static pictures, including surfaces updated in real-time.
- Simulations at the touch of a button, thanks to automatic force field parameter assignment using AutoSMILES, a new approach combining SMILES strings with RESP and AM1BCC charges.
- Extend the Twinset with your own plugins written in Python.
- Yanaconda, a uniquely simple macro language. The example below loops over all PDB files in id_list.txt and creates a table of Ramachandran plot scores assigned by WHAT_CHECK:

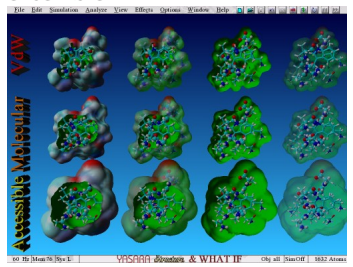
```
for id in file id_list.txt
  DelAll
  LoadPDB (id)
  Tabulate Check PhiPsi
SaveTab default,Filename=result.txt,Format=Text,Columns=1
```

Many of these features are available for free as part of YASARA View from

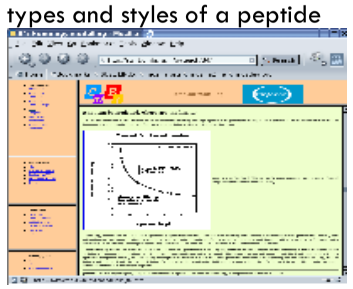
www.YASARA.org



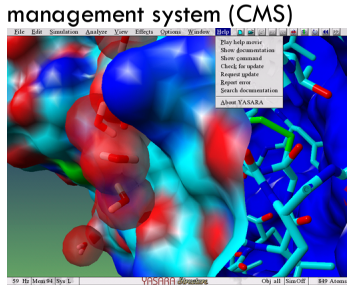
WHAT IF: NMR structure ensemble



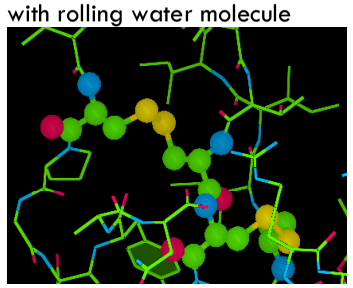
TWINSET: Various surface types and styles of a peptide



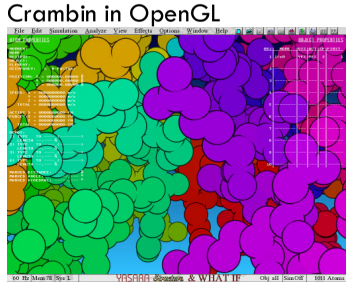
WHAT IF: The new content management system (CMS)



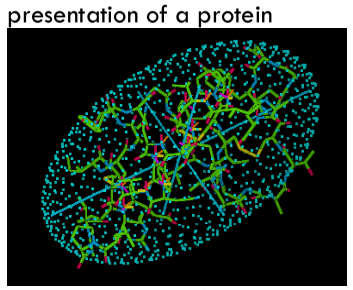
TWINSET: Molecular surface with rolling water molecule



WHAT IF: Close-up view of Crambin in OpenGL



TWINSET: Comic style re-presentation of a protein



WHAT IF: Principal axis analysis and Fibonacci ellipsoid

WHAT IF highlights

A whole series of new facilities, and even whole menus, have been added the last couple of years. The longer ago you got your WHAT IF, the more new things you will discover. Some examples are:

Electrostatic calculations

A content management system

A menu to make JMOL pages

Structure factor calculation

A GROMACS interface

The CONCOORD molecular dynamics simulation menu

Use of solid spheres

pKa calculations

Automatically 'understanding' small molecules

Multiple sequence alignment and multiple structure alignment

A menu to make representative subsets of the PDB

The WHAT IF WWW pages got revamped too. At http://swift.cmbi.ru.nl/ you find a completely reworked set of help pages, examples, figures, a WHAT IF user course, and many more.

Electrostatics. The WHAT IF electrostatics modules were designed by Jens Nielsen, now working at the University of Dublin. They provide a very (time-consuming but) precise pKa calculation method, and options to visualize electrostatic potentials.

CMS and JMOL. WHAT IF now contains a small CMS especially made for rapidly producing education web sites. WHAT IF can now produce JMOL 3D visualization pages both in the CMS and stand-alone.

Structure factor calculation was added. More X-ray options will follow.

Validation. Structure and model validation has always been an important aspect of WHAT IF. In the new version (WHAT IF 6.0), the validation menu has been improved a lot, especially the famous FULCHK option that produces extensive, human readable, validation reports has been updated and extended.

Concoord, written by Bert de Groot, is now part of WHAT IF too. It predicts the outcome of MD runs and determines macromolecular flexibility.

An interface to GROMACS, written by Olie Lange, has been added to replace the obsolete GROMOS interface.

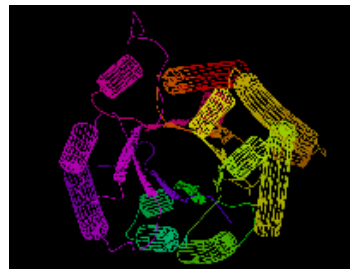
Solids. Although Yasara makes much nicer pictures, WHAT IF now also has its own solid representations. This is possible because Rolando Rodriguez rewrote the WHAT IF graphics part for OpenGL.

PRODRUG, written by Daan van Aalten, interprets small molecules and produces topology entries so that WHAT IF works better with ligands.

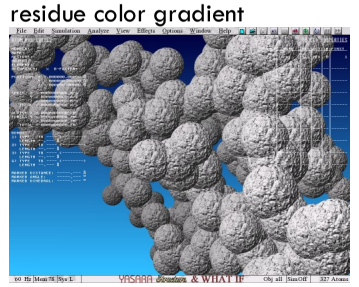
The sequence menus were originally written for the GPCRDB, but slowly are getting more general. These menus aren't very user-friendly, but do a lot of things that no other software can do with sequence families (Entropy-Variability analysis; correlated mutations, multiple sequence analysis).

Some useful WWW addresses:

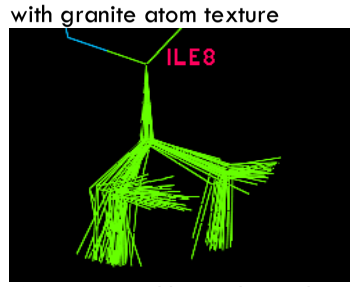
WHAT IF	http://swift.cmbi.ru.nl/whatif/
WHAT IF servers	http://swift.cmbi.ru.nl/
YASARA	http://www.yasara.org/
PDBREPORT	http://swift.cmbi.ru.nl/gv/pdbreport/
DSSP	http://swift.cmbi.ru.nl/gv/dssp/
HSSP	http://swift.cmbi.ru.nl/gv/hssp/
PDBFINDER	http://swift.cmbi.ru.nl/gv/pdbfinder/
GPCRDB	http://www.gpcr.org/7tm/
NucleaRDB	http://www.cmbi.ru.nl/NR/
KchannelDB	http://www.receptors.org/KCN/



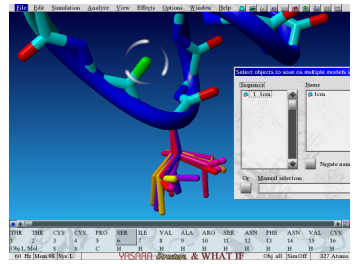
WHAT IF: TIM barrel with per-residue color gradient



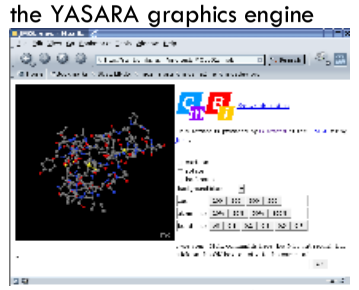
TWINSET: CPK model of 1CRN with granite atom texture



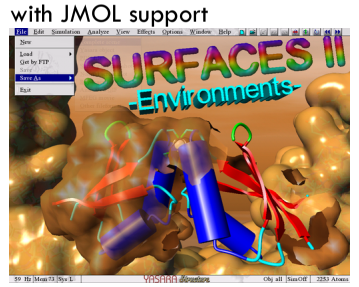
WHAT IF: Backbone dependent rotamer distribution



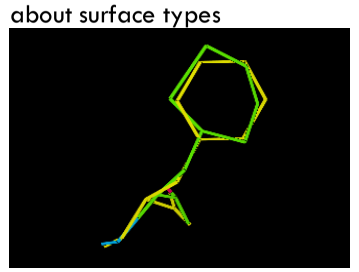
TWINSET: Same as above using the YASARA graphics engine



WHAT IF: Creating web pages with JMOL support



TWINSET: Interactive tutorial about surface types



WHAT IF: rapid regularization of structures.