**Highlights of What's New**

**Proasis3 - 2013 version**

****

**Major New Features:**

* Similarity searching has been implemented
* Any HitList can be sorted by chemical similarity
* Any HitList can be sorted by date loaded
* Enabled regnos to be shown in optimised PyMol alignments
* Improved viewing of non-bonded contacts for acceptors around metals
* Updated desolvation penaties for structures without waters, allowing penalties for only short polar-apolar contacts
* Extended PyMol scripts to include both absolute and relative b factors
* Updated MOE scripts used for visualisations
* Extended Search page to allow lists of corporate registration numbers to be copy and paste in for all browsers.
* Multiple ligands in one binding site can be displayed/managed in a single Hitlist row
* Extended database Tables to automatically store SMILES of the bound ligand, enabling this to be shown when different to the expected structure according to the entry in the corporate database
* Extended structure submission to allow strucid to be defined
* Automated ligand detection improved to better handle cases where the ligand gets put onto the end of a peptide chain, which may also include solvent molecules
* TreeView page allows for multiple selections
* Extended spreadsheet reports from SaveHitList page
* ProjPymol has many updates, including:
  + extended selection options for structure viewing
  + being able to create a combined Scorpion object for all ligands
  + builds now done in sub-directories

**Minor Enhancements and Fixes:**

* HitList rows now include additional links, with same icons as in Proasis2 hitlists
* Additional structure information available in Details section of StrucDetail page
* Session file links on StrucDetails page - View Structure Details - in links section
* Downloading selected pdb files from HitList page now provides zip file of gunzipped pdb files
* More stringent polar clash constraint used in ViewContacts
* Increase length of varchars for storing the names of software packages used during refinement
* For web-based structure submission, possibility to remove hydrogens has been depreciated
* Enhanced searching directly from a link - sequence searches can be done by prepending the query with the four characters: 'SEQ.'
* Enhanced searching directly from a link - all chains and all small molecules for a structure can be retrieved by prepending the query with the four characters: 'ALL.'
* Increased default number of rows in Hitlist page to 25
* Changed default sketcher in Seach page to JME
* Minor bug fix when updating a regno for ligands in other monomeric units
* Additional online hlep provided for addotherligand.py