The following are list of changes in PyRx version 0.5 and earlier:

**Version 0.5 - 25 March 2010**

- Added Save as Comma-Separated Values (CSV) tool for database tables.
- Added plotting feature for database tables. This feature can be accessed through a toolbar button under Tables tab. By default, it opens up Table Plotting Dialog where a bar plot of Binding Energy versus Ligand (index) is shown. If you have PubChem BioAssay opened using open CVS button, this widget will also check to see if there is Outcome column in that table, and if so, it will color bars corresponding to "Active" compound red and bars corresponding to "Inactive" blue.
  - Changed default for maximum number of energy evaluations (generic algorithm parameter in AutoDock) from medium (ga_num_evals = 2500000) to short (ga_num_evals = 250000).
- Added AutoDock PBS job submission progress dialog.
- Fixed a bug that was causing problems when displaying molecular surfaces for docked conformations.
  - Added a dialog to select alternate conformation when making macromolecule file (pdbqt) for AutoDock.
- Enabled Enthought's quality agent that can be used to get bug report and comments from a user.
  - Added Cancel option for AutoGrid Web Services.
  - Implemented flexible residues for AutoDock. This feature can be accesses by selecting residue(s) under Navigator -> Molecules and right-clicking on them. Select AutoDock -> Flexible Residues to create _flex folder under Navigator -> AutoDock -> Macromolecules with receptor pdbqt and flex.pdbqt. All docking to this receptor is then done with this flexible residue(s).
  - Updated Python to version 2.6 and ETS to 3.4.0.
  - The new installers delete previous installation folder, if any, before installing this new version.

**Version 0.4 - 2 November 2009**

- Fixed TraitError: The 'cpu_num' (see Re: PyRx won't start).
- Added AutoDockRemotePreferencesPage to allows users to change AutoDock and AutoDock service names. The defaults are set to Autodock_4.2.1 and Autodock_4.2.1.
  - Modified Remote Jobs Query in webSerives; it now updates the GUI after checking each job individually.
- Made changes to AutoDockPage to make parsing and displaying docking results faster.

- PyRx Table is populated when user clicks on that tab to speed up the startup time (see Re: How can I find the mistake).

Version 0.3 - 23 September 2009

- When making AutoDock Ligands using Open Babel, it now logs problem causing cases.

- Fixed Maximize action for Run AutoGrid page on AutoDock Wizard.

- Local AutoDock executable paths can now have spaces in it.

- Added splash screen.

- Updated Enthought Tool Suite to version 3.3.0.

Version 0.2 - 20 June 2009

- Addition of Molecular Surfaces Using IsoSurface.

- Upgraded AutoDockTools to version 1.5.4.

- Modified default Mouse Picking provided by Mayavi keyboard interactions. Pressing ‘p’ key now displays the full name and coordinates of the atom under the cursor.

Version 0.1 - 23 April 2009

- Fixed a couple of critical bugs including the one mentioned here.

- Upgraded Enthought Tool Suite to version 3.0.2 and Open Babel to 2.2.1.

- Added new AutoDock Execution Mode labeled Cluster (Portable Batch System) mode.