

XedTools 3.2.0 Release Notes

About XedTools

The XED tools are a set of command-line programs to provide modelling and cheminformatics functions using Cresset's XED force field. The current XED tool suite includes the following tools:

- XedeX
 - Generate conformations for one or more molecules
- XedMin
 - Minimise one or more molecules
- XedConvert
 - File conversion utility supporting smiles, sdf, mol2, xed and pdb files.
- Visualization Plugins
 - Plugins for popular molecular modelling applications that enable the visualization of Cresset's field points within these applications. Currently plugins for PyMol and MOE are available.

Supported Platforms

Minimum specifications

Hardware	Specifications
RAM	512MB
Processor	2Ghz Pentium 4 or equivalent
Disk space	50MB
Operating Systems	Windows 7 Red Hat Enterprise Linux 6

Recommended specifications

Hardware	Specifications
RAM	1GB
Processor	Core2Duo or better
Disk space	50MB
Operating Systems	Windows 7 Red Hat Enterprise Linux 6

Installation

Windows

Browse to the Windows folder of the distribution media and double click the "XedInstaller_<arch>_<vers>" executable file. Follow the on-screen instructions. If you have a previous version of the XED tools installed then this will be removed before installation of this version.

Linux

Browse to the Linux folder of the distribution media. Install the re-locatable rpm package using the command

```
rpm -i cresset_xed-<vers>-1.<arch>.rpm
```

Alternatively unpack the "XedTools_<arch>_<vers>.tgz" file to a suitable location (e.g. \$HOME or /usr/local or /opt). A 'cresset' directory will be created containing the tools.

Visualization Plugins

Browse to the Plugins folder of the distribution media. Load the desired plugin into the parent application. Currently plugins for PyMol and MOE are available.

MOE

Double click the supplied svl script or use the “run” command to bring in the “ReadCresset” command.

PyMol

Use the Plugin Manager to install the plugin. This enables a “Cresset” entry under the “Plugin” menu and a “load_cresset” command.

Use the tools

Windows

The XED tools require a DOS environment to run. In a DOS window type e.g.:

```
C:\Program Files\Cresset-BMD\XED\xeddex.exe -h
```

Linux

Type

```
/path_to_installation/cresset/xed/bin/xedex -h
```

where *path_to_installation* is the directory where the distribution was unpacked. If installation was from an rpm package with the default locations then the installation will be in */opt*.

Pipelining tools

Cresset provide interfaces to the XedeX and XedMin through Knime, Pipeline Pilot and Discovery Studio. Please contact [Cresset support](#) for instructions on how to download and install these interfaces.

Licensing

If you have been provided with a single-user license file from Cresset, then place it in one of the location listed at <http://cresset-group.com/license-file-locations> or in the default license locations:

- Linux: */opt/cresset/licenses*
- Windows: *C:\Program Files\Cresset-BMD\Licenses*

Change Log

New in Version 3.2.0.

New features:

- XedeX can now enumerate unspecified chiral centres
- Atoms are reordered on input to place heavy atoms before hydrogens

Improvements and bug fixes:

- Updates to ring library
- Improved ring library behaviour in XedeX
- Improved handling of Boron and Silicon
- Improved stability of SMILES generation and parsing
- Improved PDB handling (e.g. insertion codes, negative residue numbers)
- Fixed bugs on chirality handling

New in Version 3.1.0

New option in XedeX to hold bonds in input geometry during the conformation hunt enables conformation exploration of segments of molecules

New visualization tools that use the Xedconvert binary to calculate field points for a molecule and then display these in another application, currently available for PyMol and MOE.

Improved support for pdb files in Xedconvert

Improved support for molecules with unspecified chiral centres - XedeX now enumerates all unspecified chiral centres in a molecule when generating conformations.

Improved conformation hunting options and recommendations for exhaustive settings - using lower energy, highly minimized conformations results in improved reproduction of bioactive conformations

Numerous minor improvements

New in Version 3.0.0

New version of XED force field that incorporates:

- a completely analogue modelling of nitrogen geometries
- enhanced description of the electrostatic potentials around aromatic halogens
- support for some boronates and silicates

Added XedConvert binary to the distribution to aid molecule conversion from 1D, 2D or 3D formats to Cresset's xed format

Improvements to XedeX conformation hunting on ring systems with improved ring library

Introduced option to minimize ligands in a fixed protein active site using XedMin

Known Issues and Bugs

Very occasionally XedeX will fail to pop a molecule from 2D to 3D resulting in no conformations.

Occasionally XedeX will fail to correctly enumerate molecules with undefined chiral centres.

The Cresset Support Team

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