Cresset
BioMolecular Discovery Limited

XedeX

Version 1.0.0

13 April 2006

Introduction
& Installation

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Welcome to XedeX

1.1. What it does

XedeX is a program to read in one or more molecules in SDF, mol2 or XED format, perform a conformational hunt using the XED force field, and write the results to standard output. The conformational hunt process is designed to generate a highly diverse set of conformations, all of which are minimised, in as short a space of time as possible.

XedeX is designed to find a representative set of minimum vacuum energy structures using the features of the XED force field. It is not designed to find all local minima over a given energy range. Rather, it has been designed to collect as broad a range of conformationally diverse structures as possible above the global minimum. This strategy is implemented deliberately to feed the requirements of the field overlay protocols (FieldTemplater, FieldAlign etc.) which need wide sampling of conformational space.

1.2. System Requirements and Installation

XedeX is supplied as a tarball "`xedex_1.0.0.tgz`" containing 32-bit Linux binaries. It should run on any recent version of Linux (kernel 2.4 or higher, and libc6), and has been tested on Debian Sarge, Red Hat Enterprise 3, and SuSE 9. IRIX binaries are available on request. A 64-bit version of XedeX is not currently available.

XedeX can be installed either as a system-level install (for all users) or as a user-level install (in a user's home directory).

To install XedeX as a system-wide installation:

Unpack the tarball in an appropriate directory (e.g. "`/usr/local`" or "`/opt`"). A "`cresset`" directory will be created:

```
cd /usr/local
tar -zxvf xedex_1.0.0.tgz
```

Add the following lines to `/etc/cshrc` (replacing '`/usr/local/cresset`' with the actual install location):

```
setenv XED /usr/local/cresset/xed
source $XED/setupxed.csh
setenv PATH ${PATH}:$XED/bin
```

Add the following to `/etc/profile` or `/etc/bash.bashrc` (replacing '`/usr/local/cresset`' with the actual install location):

```
export XED=/usr/local/cresset/xed
source $XED/setupxed.sh
export PATH=${PATH}:$XED/bin
```

To install XedeX as a user

Copy the tarball to your home directory (or similar writable location). Unpack it and a "`cresset`" directory will be created:

```
cd
tar -zxvf xedex_1.0.0.tgz
```

If you are a csh user, add the following lines to `~/.cshrc` (replacing '`~/cresset`' with the actual install location):

```
setenv XED ~/cresset/xed
source $XED/setupxed.csh
setenv PATH ${PATH}:$XED/bin
```

Otherwise, add the following to `~/.profile` (or `~/.bashrc`) (replacing '`~/cresset`' with the actual install location):

```
export XED=~/cresset/xed
source $XED/setupxed.sh
export PATH=${PATH}:$XED/bin
```

This will add the '`cresset/xed/bin`' directory to your `$PATH` and the '`cresset/xed/man`' directory to your `$MANPATH`.

For help installing or using XedeX please contact Cresset Support at support@cresset-bmd.com.

1.3. Running XedeX

The first requirement for using XedeX is to provide a data file contain the details of a molecule. It may be noted that XedeX can be given multiple filenames which it processes sequentially. The input files can be in mol2, XED or SDF format.

The simplest input would provide an input sdf file, the standard output directed to an sdf output file and the use of all internally set default conditions;

```
xedex -v molecule1.sdf > output.sdf
```

It is recommended that the **`-v`** option generally be used, as this will result in a log of the calculation being written to standard error. The 'output.sdf' file will then contain the conformers that have been found and sorted by absolute XED force field energy values.

If you want to visualise the conformations of the molecule, then adding the **`-o x`** switch will cause the final results to be written in XED format, which can then be viewed using the supplied *xedview* molecule viewer.

For help using XedeX, see the manual (supplied in PDF format), run

```
xedex -H
```

or type

```
man xedex
```

1.4. How to get a license file

If the tarball was provided with a license file, it will already exist in `$XED/licenses` and the binaries will find it automatically. If instead you get a message about "`error checking licenses`" or "`license expired`", then please contact Cresset support (support@cresset-bmd.com) for a new license file. License files should be placed in the `$XED/licenses` directory. XedeX is commercial software and may not be used without a license. For pricing and licensing terms please contact Cresset at info@cresset-bmd.com.

A 30 day demonstration license can be obtained free of charge by visiting http://www.cresset-bmd.com/xedex_demo.html. On receipt of your demo license, copy the file to the `$XED/licenses` directory.

Please contact Cresset support if you have any other issues with the XedeX installation or operation.