

AutoDock-4.2.6 for PRIMERGY

ウェブページ

<http://autodock.scripps.edu/>

バージョン

4.2.6

ビルド環境

▶ Intel Compiler 15.0.2.164

ビルドに必要なファイル

▶ [autodocksuite-4.2.6-src.tar.gz](#)

▶ [autodocksuite-4.2.6-examples.tar.gz](#)

ビルド手順

```
#!/bin/csh -f
umask 022
unsetenv LANG
set work=/work/users/${USER}
set autodock=autodock426
set file_autodock=/home/users/${USER}/build/${autodock}/autodocksuite-4.2.6-src.tar.gz
set file_examples=/home/users/${USER}/build/${autodock}/autodocksuite-4.2.6-examples.tar.gz
#
cd ${work}
if (-d src) then
  mv src src-erase
  rm -rf src-erase &
endif
tar xzf ${file_autodock}
chmod 755 src/autodock/configure
chmod 755 src/autogrid/configure
touch src/autodock/NEWS
touch src/autogrid/NEWS
touch src/autodock/ChangeLog
touch src/autogrid/ChangeLog
sed -i 's/#define NUMG 8/#define NUMG 28/' src/autodock/ranlib.h
# --- autodock ---
cd ${work}/src/autodock
autoreconf -i
mkdir ${work}/src/autodock/x86_64Linux2
cd ${work}/src/autodock/x86_64Linux2
setenv CXX icpc
setenv CXXFLAGS -xHost
setenv CC icc
setenv CFLAGS -xHost
../configure --prefix=/local/apl/pg/${autodock}
make -j 8
make check
make install
# --- autogrid ---
cd ${work}/src/autogrid
autoreconf -i
mkdir ${work}/src/autogrid/x86_64Linux2
cd ${work}/src/autogrid/x86_64Linux2
setenv CXX icpc
setenv CXXFLAGS -xHost
setenv CC icc
setenv CFLAGS -xHost
../configure --prefix=/local/apl/pg/${autodock}
make -j 8
make check
make install
# --- examples ---
cd /local/apl/pg/${autodock}
tar xzf ${file_examples}
```