ReadMe file for: Automated molecule editing in molecular design, JCAMD 2013, submitted

The supplementary material consists of the following files:

ReadMe.pdf (the file that you are reading)

MUDO source code and makefile (you'll need a valid OpenEye license and the makefile will need some minor editing).

mudo.1.0.cpp
make_mudo
mudo.documentation.pdf

These are the files (isomeric SMILES structure format) for the pyrazole tautomer example in the article. You don't need a vector bindings for this example;

pyrazole.ism (input structures)
pyrazole.smk (SMIRKS for flipping pyrazoles)
pyrazole_enum.ism (output from enumeration)
pyrazole_enum_exhaustive.ism (output from exhaustive enumeration)
pyrazole_enum_exhaustive_canonical.ism (output from exhaustive enumeration with selection of canonical tautomer)

These are the files (isomeric SMILES structure format) for the pyrazole tautomer example in the article. The same vector bindings are used for both steps.

piperazine.ism (input structures)
piperazine.vb (vector bindings)
piperazine_prot.smk (SMIRKS for first step)
piperazine_flip.smk (SMIRKS for second step)
piperazine_prot.ism (structures from first step; use normal mode)
piperazine_prot_flip.ism (structures from second step; take structures from first step and use enumeration mode exhaustively)

Results from matched molecular pair analysis (comma-separated format)

reversed_sec_amide_mmp.txt (effect of secondary amide reversal on affinity/potency)
reversed_ter_amide_mmp.txt (effect of tertiary amide reversal on affinity/potency)
vinyl_sulfone_mmp.txt (S3 substituent MMPA of activity of vinyl sulfones against Cuzain)