

## README

### *File descriptions:*

The two directories for DIG18 and DIG20 contain the following files

- **Protein** structure as a mol2 file that was used to generate the decoy sets
- **Decoy** set as a mol2 file that contain exactly one near-native pose among 200 poses

### *Structure set-up notes for DIG18 and DIG20:*

- All structures have very high quality electron density on the ligand and active site residues to guide setup
- All histidines/glutamic acids within active site examined for most appropriate tautomeric state
- All waters and crystallographic additives removed
- N-terminus and C-terminus capped
- No broken chain in DIG18 and DIG20 found
- Residues with missing side-chain atoms were added using MOE 2011.10
  - 17 residues with missing atoms in DIG18:  
Met 1, Arg 12, Glu 29, Pro 39, Lys 42, Glu 49, Arg 56, Leu 57, glu 60, Arg 65, Asp 68, Gln 70, Glu 73, Lys 96, Gln 111, Leu 122, Arg 123
  - 33 residues with missing atoms in DIG20:  
Lys 4, Glu 5, Ile 6, Arg 12, Asp 18, Arg 20, Glu 29, Lys 42, Glu 46, Glu 49, Arg 56, Leu 57, glu 60, Tyr 61, Thr 67, Asp 68, Gln 70, Glu 73, Asp 76, Asp 78, His 90, Thr 91, Val 92, Ser 93, Lys 96, Arg 106, Asp 109, Gln 111, Leu 122, Arg 123, Glu 126, Pro 127, Leu 128
- Net charges for DIG18 and DIG20 are -4.0 and -8.0, respectively
- Partial charges added (AM1-BCC for ligand, MMFF94x for protein) using MOE 2011.10
- Hydrogens added and minimized using MOE 2011.10 (MMFF94x)
- Any residue within the active site with alternate conformations were examined manually and the most appropriate conformation kept in the coordinate file
  - For any residue outside of the active site, conformation A was retained
- Most appropriate tautomeric and protonation state were selected for the bound conformation of the ligand in the presence of protein

### *Decoy notes for DIG18 and DIG20:*

- Performed native docking using DOCK (version 6.5)
- A diverse set of 200 poses was selected using the ranking obtained from the “Diverse Subset” utility in MOE 2011.10
- To make the clear distinction between the right and the wrong decoy poses, all the poses with  $\text{RMSD} < 2 \text{ \AA}$  were discarded except for the near-native pose ( $\text{RMSD} < 1.0 \text{ \AA}$ )