The current directory contains the input file: 1\_AHRagANTcomb\_fromsmi\_nooverlap.sdf

and scripts used to run filter, omega, and ROCS (Note: These three are openeye programs and require license from OpenEye Scientific Software, Santa Fe, NM. http://www.eyesopen.com).

The final output of the ROCS runs are two .rpt files. These .rpt files are provided in the directory: ../2\_AHR\_ROCS\_output\_process/