Use the R script in this directory: AHR\_script\_process\_ROCSoutput\_to\_chemvschem\_table.R

to process the ROCS output (.rpt) files.

#-------------------------

Note-1 : To speed up calculation, we have split the query into two sets and performed two ROCS runs (check our ROCS run script in directory: ../1\_AHR\_Input\_sdf\_other\_files/AHR\_ROCS\_runscript.txt)

#--------------------------

The current R script converts the .rpt file into one chemical vs chemical similarity matrix table.

We have provided the output file (AHRall\_MATRIX\_ROCS\_merge\_FINALout.zip) from our analysis in this directory. (Note: The actual .rpt file has size >1GB and hence could not be loaded into github and we have given the output table instead)