The current directory (./3\_AHR\_MAX\_CBOS\_scores) contains the R scripts to perform CBOS analysis and also to calculate ROC AUC/Enrichment factor 10% (EF10) values for CBOS and MAX score for arylhydrocarbon receptor (AHR) data.

Script for CBOS score and AUC/EF10:

- AHR\_Script\_for\_CBOSscore\_AUC.R

Script for MAX score and AUC/EF10:

- AHR\_Script\_for\_MAXscore\_AUC.R

Output of each of these two scripts will be a table with AUC and EF10 values.

Note:

1. In order to reproduce our results we have provided the reference set and query/test set used in our screening performance evaluation as .RData file (AHR\_TRAIN\_TEST\_split.RData).

2. We have also provided the codes used to start from chemical vs chemical similarity matrix (obtained by processing ROCS output .rpt file) and get a new reference and query/test set at the end of the R script (AHR\_Script\_for\_CBOSscore\_AUC.R).