Compressed zip contains:

* CSV files for three data sets: SMRT\_excluded\_rt .csv(pubchem, rt, inchi), riken\_smiles\_rt.csv (canonical smiles with aromatic symbols and retention times), HILIC\_SMILES\_rt.csv (canonical smiles with aromatic symbols and retention times)
* RDA files for 3 data sets, list of matrices for each molecule for PLaSMA and HILIC data sets, transformed from list of matrices array for METLIN SMRT data set