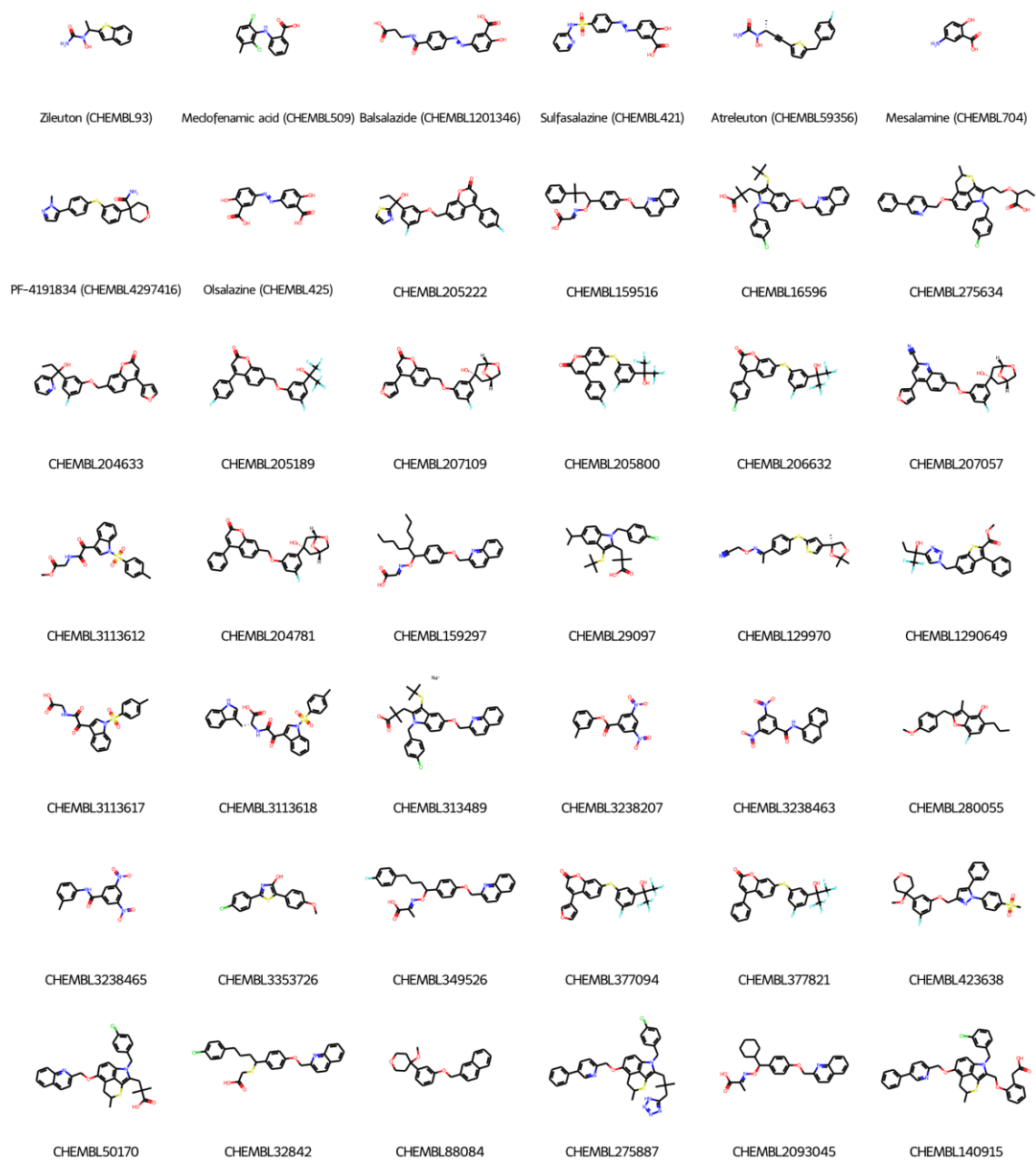


Supplementary Figure 1 - Chemical structures of all molecules extracted from ChEMBL and selected for this work.

Supplementary Figure 2 - Correlation values for several molecular descriptors calculated using RDKit, in addition to the features PLP_score, ASP_score, ChemScore and GoldScore.

Supplementary Figure 1



Supplementary Figure 2

