PSB 2018 paper: Chemical reaction vector embeddings: towards predicting drug metabolism in the human gut microbiome

Supplemental Figures

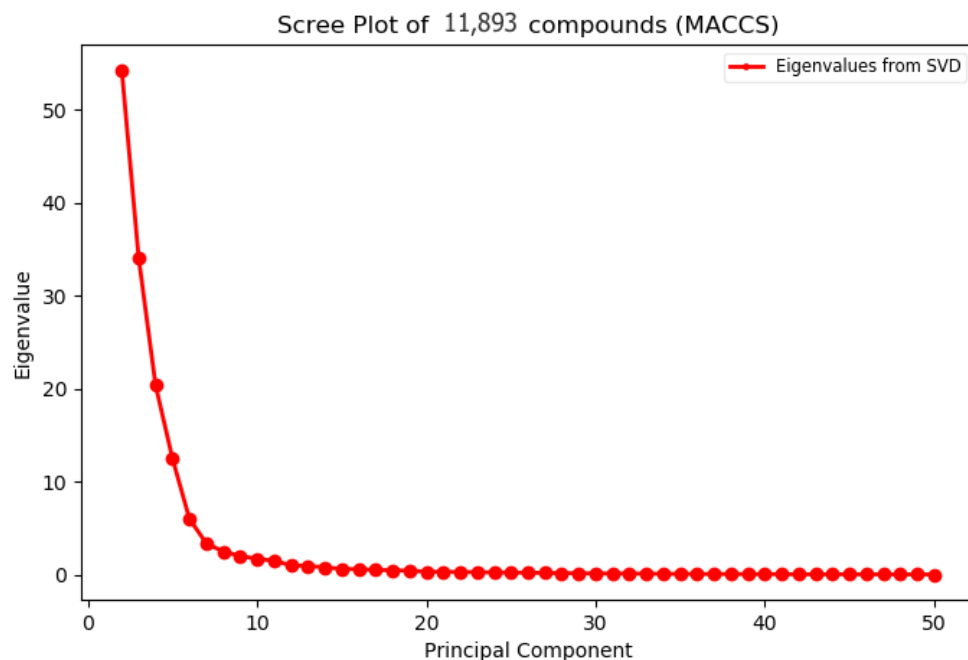
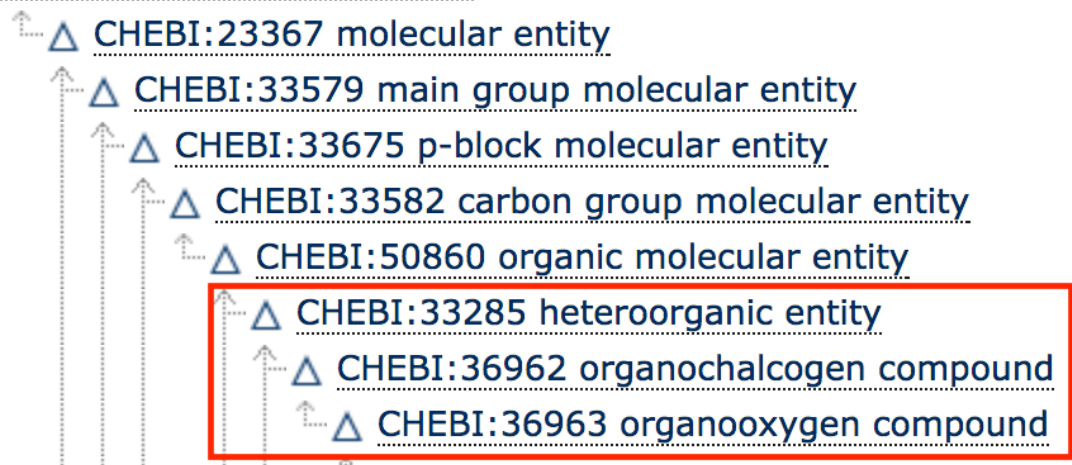Fig S1. Scree plot for the transformed vector space using 11,893 compounds.

Fig S2. Example ChEBI ontological hierarchy. The ChEBI tuple would consist of {"heterorganic entity", "organochalcogen compound", "organooxygen compound"} or using the codes 33285;36962;26963.