[P16] R-based application for a pairwise SAR analysis

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Structure-Activity Relationship Analyser is a simple tool for SAR analysis with a graphic user interface (figure 1) and a flexible approach towards the input of molecular data. The application allows calculating molecular similarity represented by Tanimoto index & Euclid distance, as well as, determining activity cliffs by means of Structure-Activity Landscape Index. The calculation is performed in a pairwise manner either for the reference compound and other compounds or for all possible pairs in the data set. The application has quantitative criteria to determine activity cliffs and their occurrence per compound with respect to SALI distribution within the dataset. The results of SAR analysis are visualized using two types of plot.

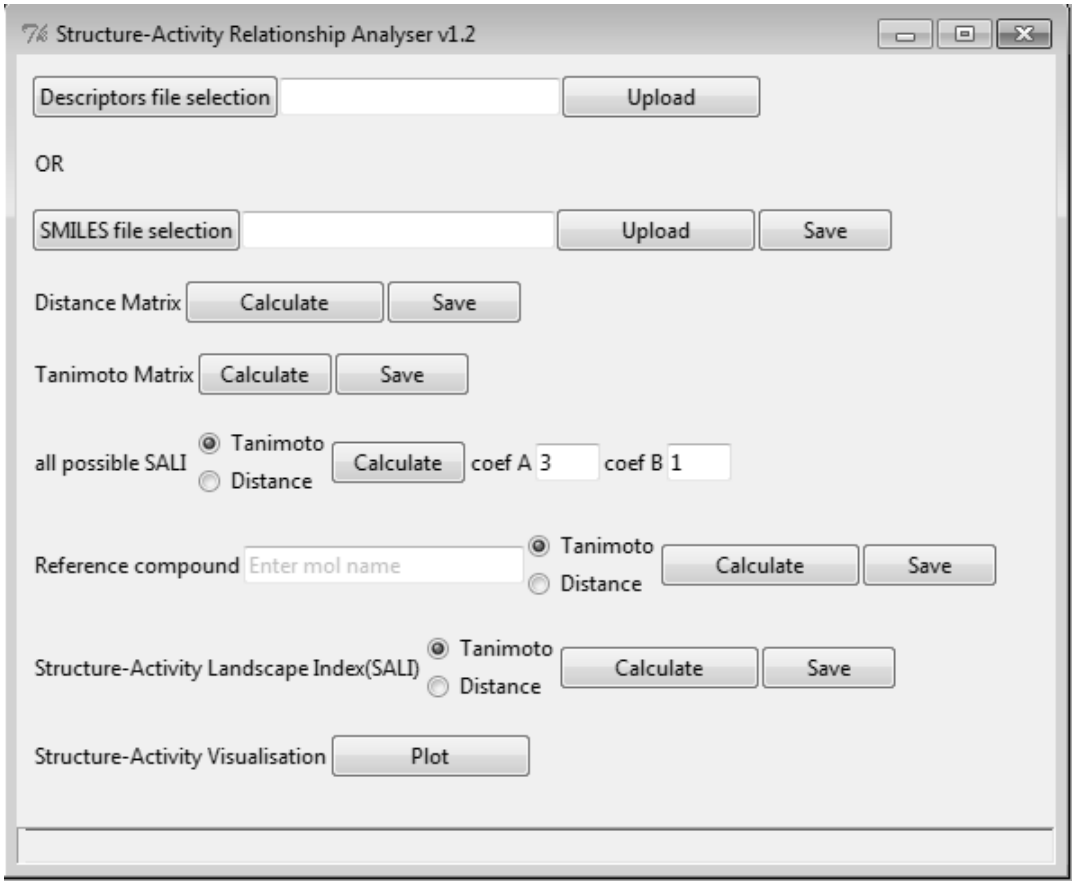

Figure 1 GUI of the application