SAS: A toolbox to represent the structure activity similarity maps for the synthesized compounds

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Background and Aims: In this study an easy to use toolbox was designed and developed to calculate and plot the structure activity similarity maps for the synthesized compounds. This tool box can be used by medicinal chemists for further studies of drug design and synthesis.
Methods: .NET programming language was used to develop a graphical interface applicable in all windows platforms (xp, vista and windows 7). The input files are entered into to the application as SMILES and Tanimoto similarity index will be calculated based on the fingerprint for each pair of compounds. The most common finger types implemented in open babel including FP2, FP3, FP4 and MACCS can be used in this step. After then the activity similarity for each pair of compounds will be calculated. A color coding system was also implemented in the application to reveal the activity range for each pair. The application was tested for two datasets including cholinesterase and betalactamase inhibitors extracted from EMBL database and its performance was validated. The input files can be easily produced using open babel package. Resutls and Discussion: The results of this study showed the applicability of this tool box in all examples. The produced data and graphs can be easily save and used in any publications.
Conclusions: Structure activity similarity maps make it possible to present a view of the chemical space and activity similarities of the synthesized compounds. It is normally anticipated that the compounds with high structural similarity exert similar activity pattern. Therefore, this view allows medicinal chemists to identify the activity cliffs in a data set and to make more rational decisions for further studies of drug design.

Keywords: Structure activity similarity map; Tanimoto index; Structural similarity