

MOEsaic: Application of Matched Molecular Pair Analysis to Interactive SAR Exploration

With the increasing size of data sets and the parallel development of multiple structural series in medicinal chemistry projects, managing and analyzing structure activity/property relationship data is becoming ever more challenging. Tools and methods for the efficient visualization, analysis and profiling of compounds therefore remain of deep interest. Here, we describe a web-based application, MOEsaic, which enhances typical medicinal chemistry workflows aimed at interrogating the SAR/SPR data through the application of interactive MMP analysis and R-group profiling.