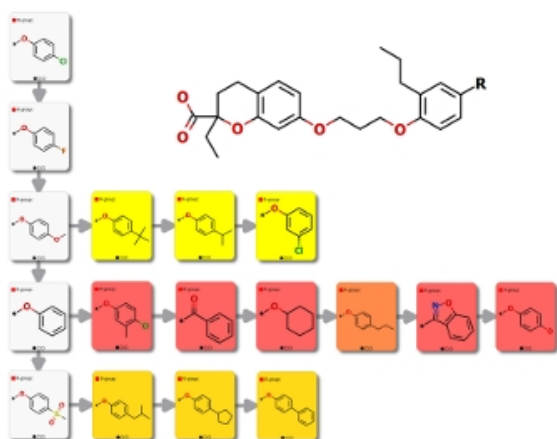


This paper, co-authored with our colleagues at [NextMove Software](#), has just been accepted for publication in Future Med. Chem. and explores applications of [Matched Series Analysis](#) to SAR transfer, binding mode suggestion, and data point validation.



### Abstract

The assumption in scaffold-hopping is that changing the scaffold does not change the binding mode and the same structure-activity relationships (SAR) are seen for substituents decorating each scaffold. We present the use of Matched Series Analysis, an extension of Matched Molecular Pair Analysis, to automate the analysis of a project data set and detect the presence or absence of comparable SAR between chemical series. The presence of SAR transfer can confirm the perceived binding mode overlay of different chemotypes or suggest new arrangements between scaffolds that may have gone unnoticed. The absence of series correlation can highlight the presence of rogue data points where assay values should be reconfirmed, or provide challenge to any project dogma.

You can download a preprint of this article as a [PDF](#) and the accompanying [Supporting Information](#)