

Structural parameters determined by supramolecular interactions in dynamic libraries

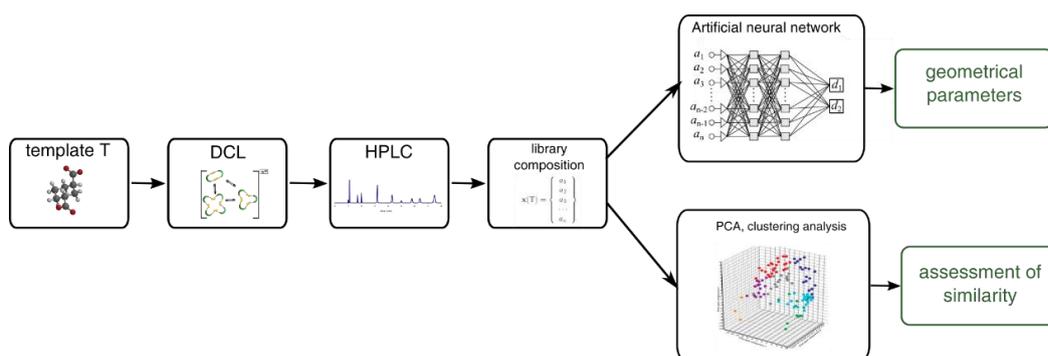
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Collective response of array of receptors can provide much information about the introduced analyte. This approach was successfully employed to simultaneously determine concentration and enantiomeric excess of chiral diols,¹ or to classify molecules according to their structural features.² Dynamic combinatorial libraries (DCL) can be treated as special class of receptor arrays, where all the receptors coexist in a dynamic mixture. In such a system the strength of interactions between receptors and analyzed molecule (template) manifest in the concentrations of library components.

In our recent papers we described a DCL of macrocyclic disulphides containing dipicolinic acid diamide.^{3,4} This DCL was found to be very sensitive to templation with oligocarboxylic acid anions. Templates of homologous series induced regular series of amplifications. DCL can distinguish between isomeric guests, including azobenzene-based photoisomers.^{5,6}

Herein we present more complex DCLs composed of multiple building blocks. The response of such libraries to introduction of various templates is analyzed by data mining tools. With this approach, certain structural aspects of templates are successfully determined and the templates can be classified according to presence of functional groups and their geometry.



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