LIFE CHEMICALS

Chemotargets

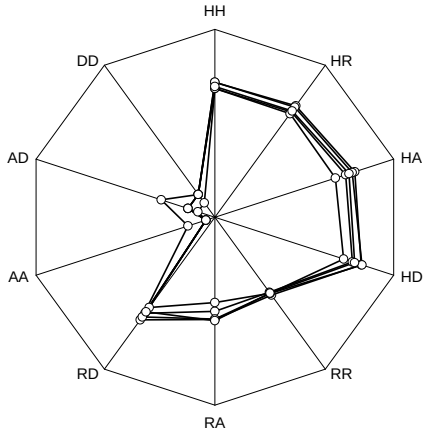
CUTE CHEMICAL LIBRARIES

Chemotargets and Life Chemicals are proud to announce their collaborative effort in the design and synthesis of a series of targeted libraries based on an innovative concept derived from SHED molecular descriptors.

Libraries targeting Nuclear Receptors, aminergic GPCR's, peptidergic GPCR's, "other" GPCR's, Serine Proteases and Kinases have already been prepared. Life Chemicals will market and sell these Libraries under the name CUTE Libraries. A great advantage of these libraries is that we can guarantee fast follow-up if hits are found.

SHED molecular descriptors

A new set of 2D pharmacophoric descriptors was recently reported (J Chem Inf Model 2006; 46: 1615-1629). Basically, SHED are derived from distributions of atom-centered feature pairs extracted directly from the topology of molecules. For the sake of simplicity, only 4 types of atomic features are considered, namely, hydrophobic, aromatic, acceptor, and donor, which give rise to 10 feature pairs.

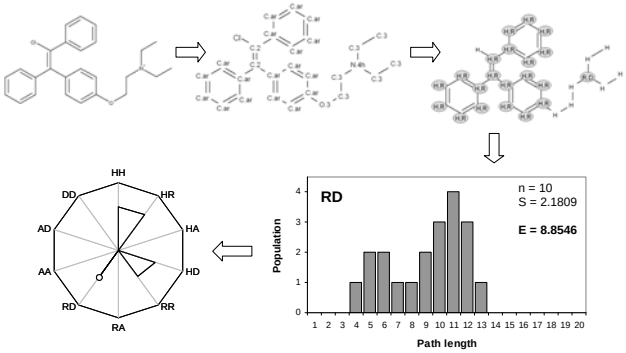


The CUTE concept

Traditionally, targeted chemical library design has focused on the selection of compounds constrained to some physico-chemical property ranges or privileged substructures observed in known bioactive compounds for the protein family being targeted. Actual coverage of the protein family has not been addressed properly. CUTE targeted chemical libraries offer fully covered, unbiased, targeted and enriched selections of compounds towards the main protein families of therapeutical relevance (J Chem Inf Model 2006; 46: 2725-2736).

Introducing CUTE Chemical Libraries

Chemotargets provides a new concept in targeted chemical library design in which chemical scaffold diversity is balanced against the pharmacological coverage of the entire chemical library over a given protein family.



Biological relevance of SHED

It was shown that bioactive compounds having similar features arranged in a similar way displayed also a similar profile of SHED descriptors. The ensemble of SHED profiles for a set of bioactive molecules can then be taken as a ligand-based description of proteins. Under this approach, the SHED of a molecule can be compared against the SHED profiles associated to a protein target. If sufficiently similar, the molecule will then receive a biological annotation.