ISIDA Fragments

ISIDA Fragments is a category of fragments descriptors. They use 2D Lewis graph representation of the compounds but do not consider stereoisomerism. They also are tautomer- and mesomer-dependant.

ISIDA Fragments uses three modes of fragmentations, corresponding to exploration of the graph representation of the molecule:

- Paths: the enumeration of all the shortest paths between any two nodes of the graph
- Trees: the enumeration of trees centered on each atom of the molecule, a tree being the concatenation of all shortest paths starting from a given atom.
- Neighbours: the enumeration of neighborhoods of each atom, a neighborhood being the concatenation lists of atoms at increasing distance from a given atom.

These fragmentation modes are completed by several representations of the atoms of the molecule:

- symbols: the atom's names are used
- pharmacophore: atom's names are replaced by pharmacophoric labels
- bonds/atoms representations can be ignored
- bond types describing creation, order change or deletion of chemical bonds are supported

The software is still under development so this short description is going to change.