Use of Artificial Intelligence in Designing Dyes, Chemical Auxiliaries, Polymers and Textile Fibers

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Each molecule is described by a set of structural features, a set of physical properties and the strength of some activity, such as toxicity. We are using artificial intelligence to find patterns of these structural features and properties that correspond to a desired level of activity in various classes of molecules. Specifically, we are:

- using genetic algorithms, neural networks and fuzzy logic along with molecular orbital methods to design dyes, chemical auxiliaries, polymers and fibers
- investigating novel molecular indices to be used for the prediction of various physical and toxicological properties of textile chemicals
- developing the machine learning (soft computing) techniques required to extract and utilize the information.

Molecular Modeling

Using density functional calculations we are establishing properties of various molecules of interest to the textile industry, initially for nontoxic azo dyes. This approach uses non-local corrections for the functional calculations1,2,3 and a numerical basis set which is very flexible and includes polarization functions on all atoms1 leading to complete geometric optimization with no constraints. We now have complete geometric optimizations of over 120 azobenzene derivatives and have calculated the following properties: atomic charges, dipole moments, highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies, and the logarithm of the octanol water partition coefficients. We now have high-quality graphical displays of the density, HOMO, LUMO and electrostatic potential for all these molecules (See Sample Graph).

Soft Computing

We are currently using three methods of machine learning: fuzzy neural tree induction,4 fuzzy logic (CUBICALC) and supervised neural network (Ward Systems Group) (See Figure below). These methods differ both in the learning strategy employed to structure the knowledge, and in the representation of the knowledge acquired by the system. Using such artificial intelligence programming language strings, we can represent backbones and side chain groups. Our techniques enable sophisticated calculations to be performed on large molecules at relatively low cost. While these three methods have successfully established predictive patterns for our databases, we have observed some limitations, particularly concerning predictions made on closely related molecules such as 2- and 3-methoxy-4-aminoazobenzene, where the calculated physical properties and topological indices are very similar, despite radically different mutagenic behaviors. We are continuing to develop our methods to account for these limitations.

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Industry interactions: I [International Pigments and Photochemicals Ltd., Canada]

Project Web Site Address:
http://titan.philau.edu/~les/

For Further Information:
4. Spartan v. 5.0 molecular modeling package (Wavefunction, Inc.).

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