VisiQuest™ Chemoinformatics Toolkit

CHEMOINFORMATICS TOOLKIT BASED ON MESA ANALYTICS & COMPUTING

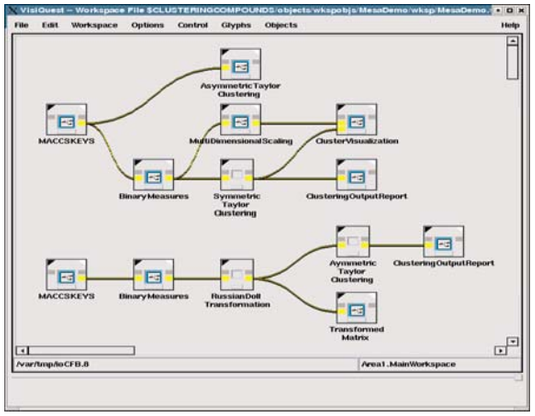

FIGURE 1
The Grouping Module contains clustering algorithms that use the visual programming paradigm of VisiQuest.

AccuSoft has partnered with MESA Analytics & Computing to bring you a leading-edge VisiQuest Chemoinformatics toolkit.

The new Chemoinformatics toolkit enables you to quickly prototype and perform:

› Similarity Searching

Use MDL MACCS Key Fingerprints and translate SMILES. Similarity Searching with the Tanimoto, Cosine, Euclidean, Hamman, or Tversky similarity or dissimilarity measures.

› Clustering

Clustering large datasets, either non-overlapping or overlapping clusters, with the Tanimoto, Tversky, Euclidean, and other measures.

› Cluster and Active Compound Inspection

Use ChemTattoo(TM) to identify substructure commonalities among a group of compounds with key-based fingerprints.

› and more ...

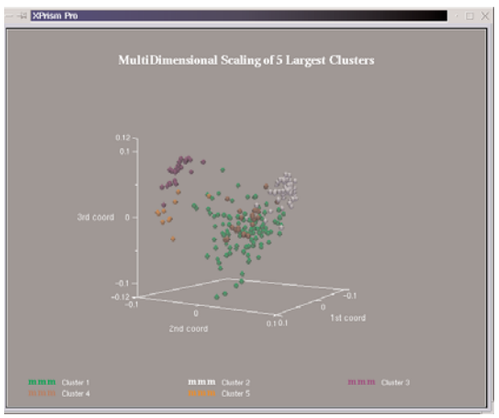

FIGURE 2
VisiQuest is readily used for the processing and exploration of multi-dimensional data. The Chemoinformatics toolkit contains a tool that determines ambiguity indices, enabling the user to find similarity thresholds that produce the least clustering ambiguity.

Chemoinformatics Toolkit Contents

Grouping and Clustering Optimized for High-Throughput Screening

VisiQuest provides a simple visual programming environment to analyze data and images which gives the user access to all of its powerful functions and algorithms at the click of a button. With the new Chemoinformtics toolkit based on state-of-the-art MESA Analytics & Computing technology, users are given access to an additional set of powerful data mining solutions that cover a variety of early drug discovery data analysis techniques.

Chemoinformatics Toolkit Functionality:

› MDL MACCS Key Fingerprints, 164 bit or 320 bit versions. Manipulate SMILES linear notation for database similarity searching, clustering, diversity, QSAR, & more.

› Similarity Searching Measures: Tanimoto, Cosine, Euclidean, Hamman, Tversky, or composite similarity or dissimilarity measures.

› Clustering measures output Ordered Pair, Sparse Matrix, or Square Matrix.

› RussianDoll. Takes as input an asymmetric matrix and outputs a transformed asymmetric matrix that groups like sub-features. Useful in structural and shape clustering for lead hopping. This algorithm is unique to Mesa.

› Additional Clustering allows for fast, space efficient clustering of very large data sets:

- Non-overlapping or overlapping symmetric clustering using Taylor-Butina algorithm with ambiguity measures
- Non-overlapping or overlapping asymmetric clustering using Taylor-Butina algorithm with ambiguity measures
- Non-overlapping or overlapping symmetric clustering using K-means with ambiguity measures
- Non-overlapping or overlapping symmetric clustering using K-modes with ambiguity measures
- Reciprocal Nearest Neighbor implementations of non-over lapping, symmetric Wards, Complete Link, and Group Average algorithms with ambiguity measures
- Non-overlapping or overlapping symmetric clustering using Jarvis-Patrick algorithm with ambiguity measures.

› ChemTattoo (TM) identifies substructure commonalities among a group of compounds with key-based fingerprints. Generates the atom counting and coloring display information and produces a collection of important modal statistics. Visualization of the structures can be performed by numerous atom coloring depicters.

› Chemical Diversity algorithm, a hybrid exclusion region algorithm that takes into account similarity measure distributions, useful in compound selection in building compound libraries.

› MDS for cluster and diversity analysis visualization.

› And much more!

For more information or a free trial, visit us at www.accusoft.com

ACCUSOFT CORPORATION 71 LYMAN STREET NORTHBOROUGH MA 01532 DOM 800.525.3577 508.351.9092 508.351.9086 FAX