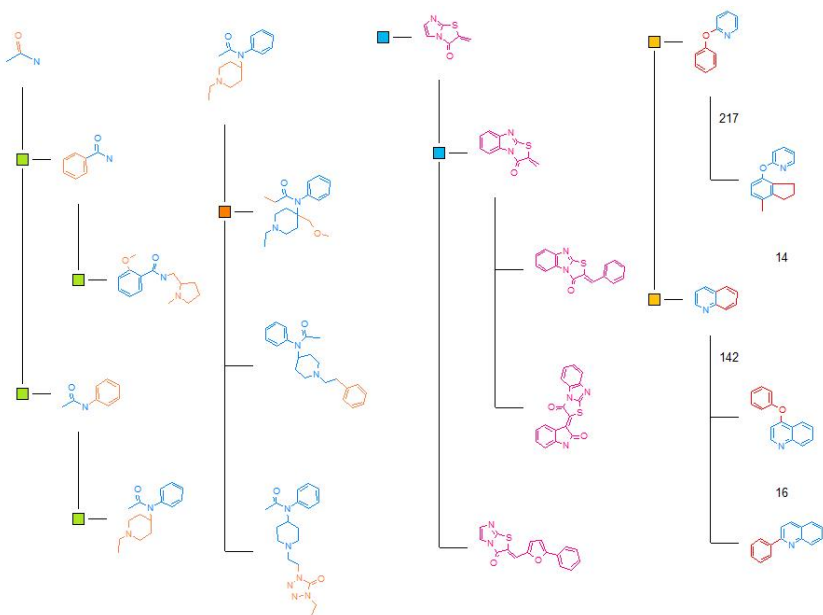


CHEMASP



AUTOMATED SCAFFOLD PERCEPTION

Server Solution for
large datasets

- Command line driven, allows integration with third party piping programs
- Drive scaffold identification through multiple user controlled specifications
- Hierarchical organization of scaffolds
- Outputs analysis in **SARvision** or SD format
- Easy to embed in internal applications

CHEMASP is a proprietary scaffold identification algorithm that identifies common substructures present in the dataset and presents them into a hierarchical tree of increasing complexity.

From an atom-by-atom scaffold expansion approach, to the use of knowledge based chemical intelligence to identify common substructures, the user has great flexibility to mine their datasets with this tool to their particular ends.

Implemented in 32 or 64 bit versions for Linux (Suze or RedHat) or Windows servers, this is a solution for large datasets fully compatible with **SARvision**.

```
Strict Match = 0;           # set this to 0
Partial Resonance = 1;     # set this to 1.
BuildAll = 1;              # Build all layers
Minimum Threshold = 3;    # smallest family
Sampling Size = 100;      # dataset sampling
Delete Trivial = 1;       # no trivial
ID Relevant Chains = 1;     # acyclic fragments
Atom By Atom = 0;         # build atom by atom
SimplifiedRingsOnly = 0;
Name Scaffolds = 1;       # Autaname scaffolds
Name Scaffolds(uniquely) = 0;
#Name Field = "ID";       # Name Field for sdf
InputSDF = "./LibraryExample.sdf";
Name Field = "MID";
```

For additional information visit our website www.ChemApps.com
Or Contact us at info@altoris.com