Software SubMat

Calculation of binary substructure descriptors

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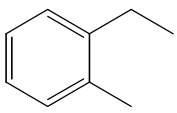
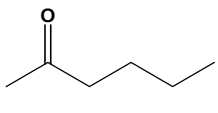
K. Varmuza
Laboratory for Chemometrics
Institute of Chemical Engineering, Vienna University of Technology
Getreidemarkt 9/166-2, A-1060 Vienna, Austria
kvarmuza@email.tuwien.ac.at http://www.lcm.tuwien.ac.at

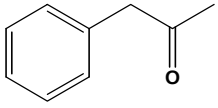
Demo Example

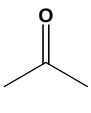
1. Preparation of two structure files *.SDF (Molfile format) by an appropriate structure editor or another software (not included in SubMat).

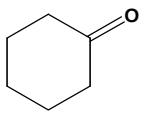
File Demo-Molecules.SDF contains 5 structures; they will be considered as molecular structures; free valences are interpreted as H-substituted.


1


2

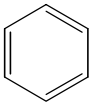

3

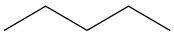

4


5

File Demo-Substructures.SDF contains 3 structures; they will be considered as substructures; free valences can be attached to any atom.


1


2


3

2. Start of SubMat.

Loading of files Demo-Molecules.SDF and Demo-Substructures.SDF.
Input of a name for the output file, for instance DemoResult.TXT.
Eventual selection of output file format. Default is "delimited by comma", optional are "delimited by blank" or "no delimiter".
Start ("Calculation of S-Matrix").

3. The generated output file DemoResult.TXT in this example is

```
0 1 0
1 0 1
1 1 0
1 0 0
1 0 1
```

Each molecular structure corresponds to one row (line).
Each substructure corresponds to one column.
A "1" indicates that the substructure is contained in the molecular structure.
For instance molecular structure 2 contains substructures 1 and 3.