Introduction

The maximum common substructure (MCS) of two molecules is the largest substructure present in both structures. The MCS characterizes an aspect of molecular similarity. SubMat determines the MCS of two chemical structures for most practical cases [1].

For a set with $n > 2$ structures the MCS of all structures may be very small and not representative for the structure set. SubMat determines the MCS for each structure pair and then ranks the MCSs by considering the size of the MCS and the frequency of presence in the n structures [2].

Input for SubMat is an SDF-file; output is an SDF-file with the found MCS(s). The isomorphism for the MCS can be adjusted (atom and bond types considered or skeleton used, minimum size and ranking of MCS).

[1] Scsibrany H., Varmuza K.: Software-Entw. in der Chemie **7**, Ges. Deutscher Chemiker, Frankfurt a. M., p.77 (1993)
[2] Varmuza K. et al.: J. Chem. Inf. Model. **38**, 420 (1998)

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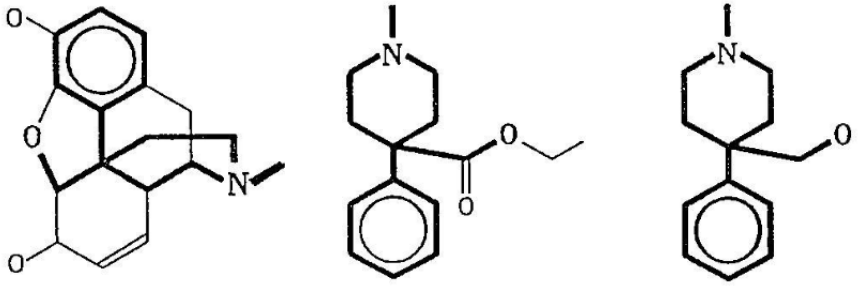
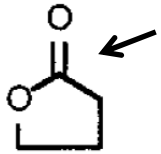
Example: MCS for two structures [1]

morphine with the MCS marked pethidine MCS (by SubMat)



Example: Hitlist from IR-spectral search [2]



Query ("unknown"), butyrolacton
Library: 13484 IR spectra
(query excluded, 3700 - 500 cm^{-1} used).
Hitlist: 50 hits with most similar IR spectra.
Evaluation by SubMat: **10 MCS**, in 46 - 28 hits; **Y**, MCS present in query structure.