

C. Compound format exchange: PDB MDL Mol and SYBYL Mol2 with CORINA 3.0

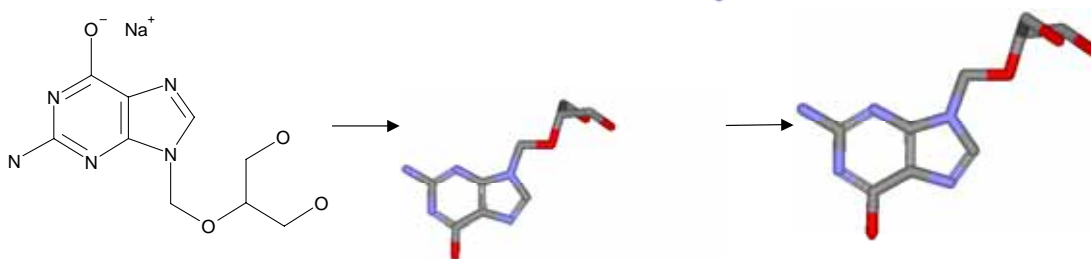
CORINA is a command line oriented program. Therefore, it has to be executed in a UNIX (Linux) shell (e.g., csh, tcsh, or bash) or, in a MS DOS shell on Windows platforms.

The general synopsis for using CORINA is:

```
corina [ -option(s) [suboption[=value],...] ] [ infile ] [ outfile ]
```

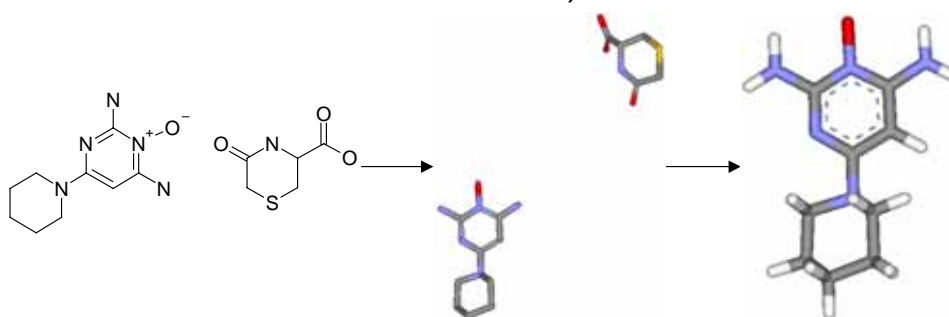
Infile and outfile are the input and output file names. If no file names are given, the program reads from standard input and writes to standard output. If only one file name is given, this file will be read as input file and the output will be written to standard output. By default, a minimum of trace output is by written to the file corina.trc. For example,

```
corina -i t=sdf -o t=sdf -d rs 145462.mol m145462.mol
```



A

```
corina -i t=sdf -o t=mol2 -d wh,rs 149015.mol 149015.mol2
```



B

- Example A: the command could remove the sodium ion from “145462.mol” and save to ”m145462.mol”.
- Example B: the command could remove the solvent molecule, add hydrogen atoms from “149015.mol” and transfer to “149015.mol2”.