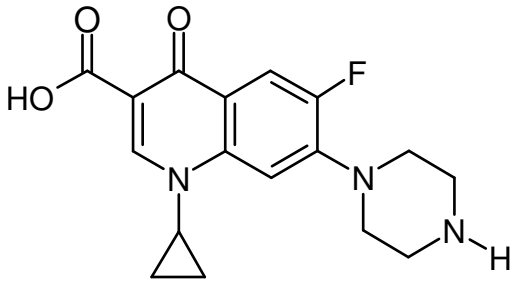
Hands-on exercises to the lecture „Modern Methods in Drug Discovery“ WS14/15

04.12.13

1. From the large class of quinolone antibiotics the most frequently administered one, ciprofloxacin is shown below



The SMILES of ciprofloxacin and further „floxacines“ are given in the file Floxacines.smi
In the CIP-Pool open a terminal window and change your directory to:

```
cd ../mihu004/bin/bin
```

The SMILES and compounds are in the text file: `Floxacines.smi`

To perform queries with SMILES/SMARTS we use the command obgrep of Open Babel:

`./obgrep "[N;H1]C(=O)" Floxacines.smi` print all molecules that contain a peptide linkage

`./obgrep -c "C(=O)O" Floxacines.smi` print only the number of matching molecules

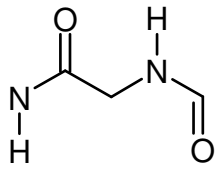
`./obgrep -v "C(=O)O" Floxacines.smi` invert matching, print non-matching molecules

Which compounds contain chlorine? (search for chlorine)

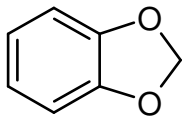
Which compounds do not contain fluorine? (inverted machting for fluorine)

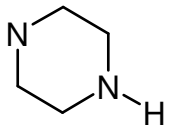
How many compounds do not contain any halogens (F, Cl, Br, I)? (logical or)

Which compound(s) contain a dipeptide linkage ? (specify the precise number of hydrogens on the nitrogen atoms)



Wow many compounds contain a 5-membered ring? (search for ring size)

Which compounds contain this fragment  ?

Which compounds contain this fragment  ?

What do following SMARTS mean? Draw matching structures.

[CH2;R0]

[OX2]

[CX4][NH2]

Construct a SMARTS string that matches as many as possible compounds and includes the following fragment (assume that both rings are aromatic):