

```
### Modul 1: Molvægts beregner
```

```
def MV (H, C, O, N, Cl, F, S):  
    hydrogen = 1.008  
    carbon = 12.011  
    oxygen = 15.999  
    nitrogen = 14.007  
    chlor = 35.450  
    flour = 18.998  
    svovl = 32.066  
    molvægt = H*hydrogen + C*carbon + O*oxygen + N*nitrogen + Cl*chlor + F*flour + S*svovl  
    return molvægt
```

```
# Beregn molvægt af atorvastatin, metformin og penicillin V  
mv_koffein = MV(C=8, H=10, O=2, N=4, Cl=0, F=0, S=0)  
mv_atorvastatin = MV(C=33, H=35, O=5, N=2, Cl=0, F=1, S=0)  
mv_penV = MV(C=16, H=18, O=5, N=2, Cl=0, F=0, S=1)  
print('koffein:', mv_koffein, 'atorvastatin:', mv_atorvastatin, 'penicillinV:', mv_penV)
```

```
koffein: 194.194 atorvastatin: 558.6500000000001 penicillinV: 350.395
```

```
### Modul 3: Mol- og koncentrationstrekanten
```

```
def mol_trekant(m, n, M):  
    if m==0:  
        masse = n*M  
        return 'masse i (g):', masse  
    if n==0:  
        mol = m/M  
        return 'antal mol:', mol  
    if M==0:  
        molvægt = m/n  
        return 'molvægt i (g/mol) :', molvægt
```

```
def koncentrations_trekant(n, c, v):  
    if n==0:  
        mol = c*v  
        return 'antal mol:', mol  
    if v==0:  
        vol = n/c  
        return 'volume i (l):', vol  
    if c==0:  
        konc = n/v  
        return 'koncentration i (mol/l) :', konc
```

```
# Opgave 3.1
n_ator = mol_trekant(m=0.010, n=0, M=558.650)
print('atorvastatin:', n_ator)

# Opgave 3.2
n_penV = mol_trekant(m=0.050, n=0, M=350.395)
print('PenicillinV', n_penV)
```

```
atorvastatin: ('antal mol:', 1.7900295354873356e-05)
PenicillinV ('antal mol:', 0.00014269610011558386)
```

```
c_penV = koncentrations_trekant(n=0.000143, c=0, v=0.001)
print('PenicillinV (mol/L):', c_penV)
```

```
PenicillinV (mol/L): ('koncentration i (mol/l) :', 0.14300000000000002)
```

Modul 4

```
#Opgave 4.1
benzylalkohol = MV(C=7, H=8, O=1, N=0, Cl=0, F=0, S=0)
hydroxybenzylalkohol = MV(C=7, H=8, O=2, N=0, Cl=0, F=0, S=0)
print('benzylalkohol:', benzylalkohol, '4-hydroxybenzylalkohol', hydroxybenzylalkohol)
```

```
benzylalkohol: 108.13999999999999 4-hydroxybenzylalkohol 124.139
```

```
### Modul 4
```

```
#Opgave 4.1
```

```
benzylalkohol = MV(C=7, H=8, O=1, N=0, Cl=0, F=0, S=0)
hydroxybenzylalkohol = MV(C=7, H=8, O=2, N=0, Cl=0, F=0, S=0)
print('benzylalkohol:', benzylalkohol, '4-hydroxybenzylalkohol', hydroxybenzylalkohol)
```

```
benzylalkohol: 108.13999999999999 4-hydroxybenzylalkohol 124.139
```

```
# LogP beregner
```

```
import math
```

```
def logP(l, h, logP):
    if l==0:
        lipofil_fase = (10**logP)*v
        return 'm(stof) i den lipofile fase er', lipofil_fase
    if h==0:
        hydrofil_fase = o/(10**logP)
        return 'm(stof) i den hydrofile fase er', hydrofil_fase
    if logP==0:
        logp = math.log10(l/h)
        return 'logP =', logp
```

```
### Bestem logP for et givent stof X, hvor der er 6.3 mg i den lipofile fase og 0.63 i den vandige fase. Volumen af de to faser er lige store.
logP(6.3, 0.63, 0)
```

```
('logP =', 1.0)
```

Modul 5: Molvægt af paracetamol og ciclosporin

```
mv_paracetamol = MV(C=8, H=9, O=2, N=1, Cl=0, F=0, S=0)
mv_ciclosporin = MV(C=62, H=111, N=11, O=12, Cl=0, F=0, S=0)
print('paracetamol:', mv_paracetamol)
print('ciclosporin:', mv_ciclosporin)
```

```
paracetamol: 151.165
ciclosporin: 1202.635
```