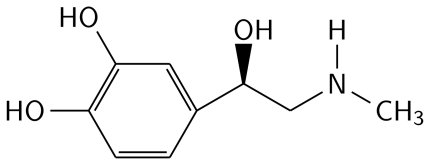
Exercise sheet 3: Reactions, dynamics, enzymes

Organic chemistry for bioinformatics, lecture 3. Exercises marked *(bonus)* are optional.

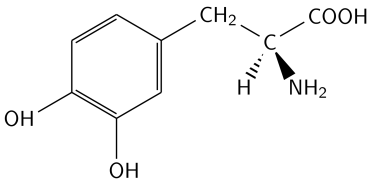
- **Check yourself**: in exercise 1 PubChem tells you R or S, and in exercise 4 your program must reproduce the numbers of exercise 3.
- **Exercise 4 needs a computer.** Use Python or any language you like; plots are welcome but not required.
- **Exercise 5 is self-study.** It is about part F of the lecture (lactase, antibiotics, aspirin), which we did not reach in class. Read the slides first.

Exercise 1: R or S?

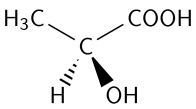
Assign **R** or **S** to the stereocentre of each molecule. Write down the priorities 1–4 of the four groups first. Then look the molecule up in PubChem (by name) and compare with the R/S label in its IUPAC name.



a) adrenaline



b) L-DOPA



c) L-lactic acid

Exercise 2: Counting with moles

Ethanol is burnt to carbon dioxide and water (in a flame, and overall also in your body):

$$C_2H_5OH + O_2 \longrightarrow CO_2 + H_2O$$

Use the molar masses C 12, H 1, O 16 g/mol.

a) Balance the equation. Count each kind of atom on both sides to check it.

b) Calculate the molar masses of ethanol, O_2, CO_2 and H_2O.

c) How many grams of O_2 are needed to burn 46 g of ethanol, and how many grams of CO_2 and H_2O are formed? Check that the mass is conserved.

d) A glass of wine contains about 10 g of ethanol. How many mol is that, and how many ethanol molecules? ($1\ \text{mol} = 6.022 \times 10^{23}$ particles)

Exercise 3: An equilibrium on paper

For the ester of the lecture, acid + ethanol $\rightleftharpoons$ ester + water, the equilibrium constant is $K \approx 4$ (lecture, slides 10 and 11).

a) You start with 1 mol acid and **3 mol** ethanol (no ester, no water). How much ester is present at equilibrium? Set up the table of slide 11, put it into K, and solve the quadratic equation. Which of the two solutions makes sense, and why?

b) Compare with the 1 : 1 mixture (2/3 mol ester). Why does an excess of ethanol help?

c) Calculate ΔG° of the reaction from $K = 4$ with $\Delta G^\circ = -RT \ln K$ ($R = 8.314$ J/(mol·K), $T = 298$ K). Is the reaction strongly or weakly downhill?

d) An acid catalyst (or an enzyme) is added to the mixture of a). Does the amount of ester at equilibrium change? What changes?

Exercise 4: Simulate the equilibrium

The curves on slide 10 come from a small program (slides 12 and 13). Write it yourself. With mass-action kinetics, the rates are $v_f = k_f$ [acid][ethanol] and $v_r = k_r$ [ester][water], and in each small time step Δt the ester concentration changes by $\Delta t \cdot (v_f - v_r)$ (Euler step). Acid and ethanol decrease, ester and water increase by the same amount.

a) Simulate the 1 : 1 mixture with $k_f = 1$, $k_r = 0.25$, $\Delta t = 0.01$, from $t = 0$ to $t = 6$. Plot (or print) the ester concentration. Do you reach 2/3?

b) Change the start to 1 mol/L acid and 3 mol/L ethanol. Does your program reproduce the result of exercise 3a?

c) Simulate a catalyst: multiply *both* rate constants by 10. What changes, what stays? (You may need a smaller Δt.)

d) Repeat a) with $\Delta t = 0.5$, 1 and 2. What goes wrong, and why?

e) *(bonus)* A pathway: A $\rightarrow$ B $\rightarrow$ C with $v_1 = k_1$[A] and $v_2 = k_2$[B], start with [A] = 1. Compare $k_1 = 0.3$, $k_2 = 3$ with $k_1 = 3$, $k_2 = 0.3$. When does the intermediate B pile up? In the adrenaline pathway the first step (tyrosine $\rightarrow$ L-DOPA) is the slow one: what do you expect for the amount of L-DOPA in the cell?

Exercise 5: Self-study: what enzymes make possible

Read the slides of part F (slides 30–32) and answer in one or two sentences each.

a) Which bond does lactase split, and what is the reaction type? To which EC class (slide 22) does lactase belong?

b) Why do people without lactase get symptoms, although the lactose itself does no harm?

c) Why is the β-lactam ring of penicillin more reactive than an ordinary amide?

d) Aspirin is an ester. What does it do to cyclooxygenase, and why does one dose act on platelets for about a week?

e) Sulfonamides block folate synthesis. Why do they harm bacteria but not us?