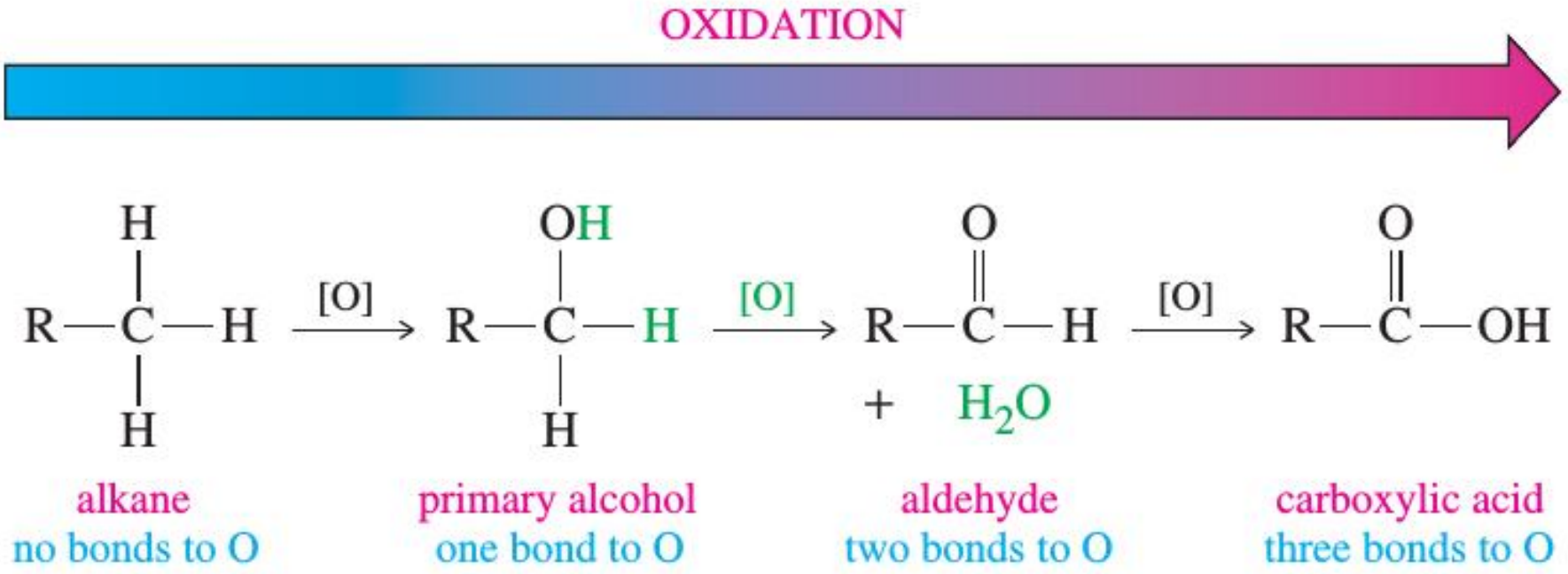
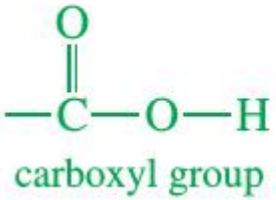
Karbonsavak és származékaik

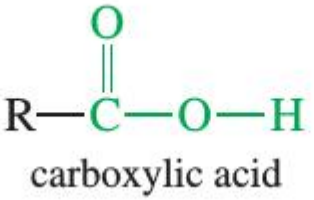


Karbonsavak

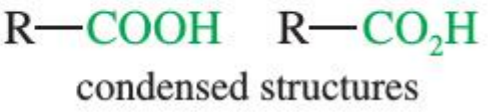
A karbonsavak funkciós csoportja a **karboxilcsoport:**



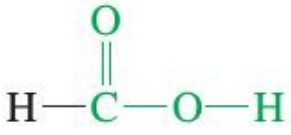
karboxilcsoport



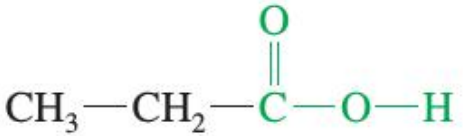
karbonsav



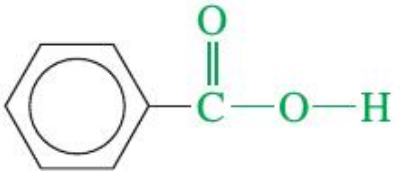
összevont csoportjelöléssel



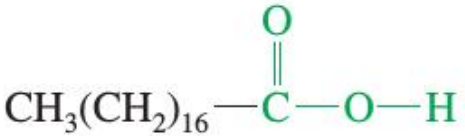
hangyasav



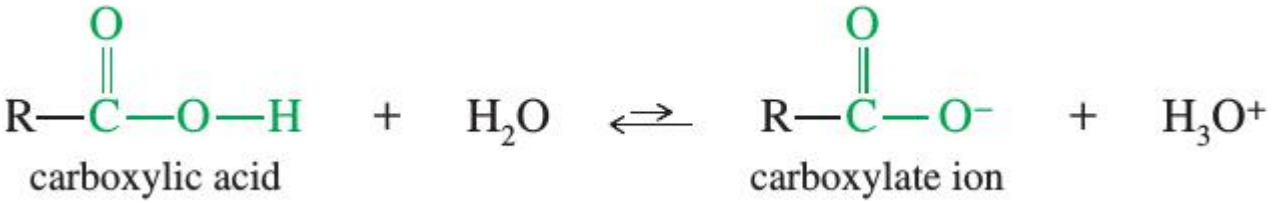
propionsav



benzoesav

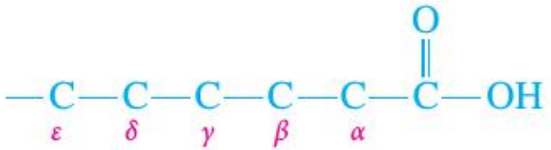


sztearinsav

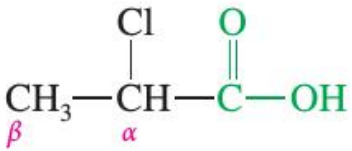


karboxilát ion

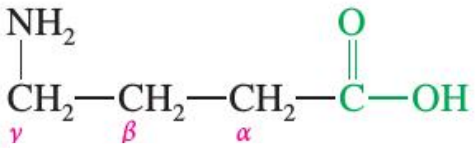
Karbonsavak szénatomjainak számozása



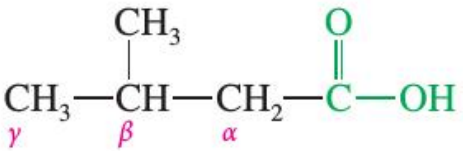
Az α helyzetű szénatom a karboxilcsoporttal szomszédos szénatom!



α-chloropropionic acid

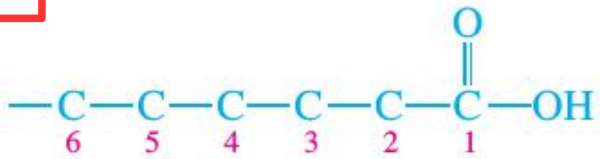


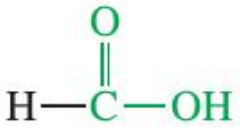
γ-aminovajsav
(GABA)



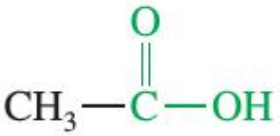
isovaleric acid
(β-methylbutyric acid)

Az 1. szénatom a karboxilcsoport szénatomja, a névbe is belevesszük!

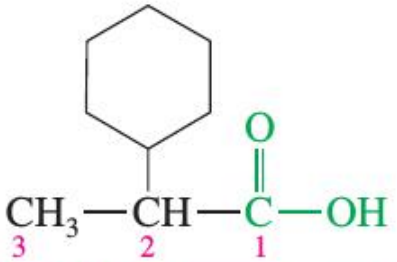




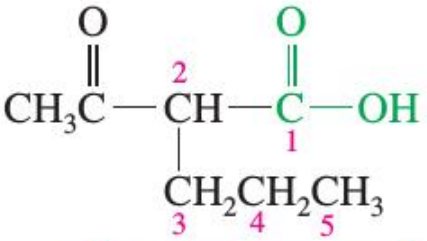
IUPAC name: methanoic acid
common name: formic acid



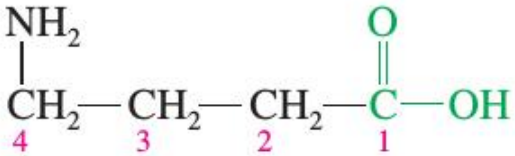
etánsav
(=ecetsav)



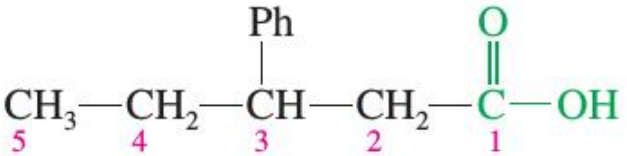
2-cyclohexylpropanoic acid
α-cyclohexylpropionic acid



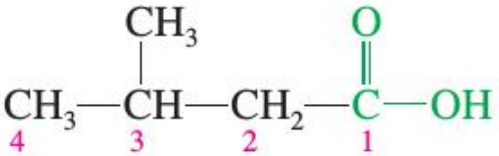
2-acetylpentanoic acid
α-acetylvaleric acid



IUPAC name: 4-aminobutanoic acid
common name: γ-aminobutyric acid



3-phenylpentanoic acid
β-phenylvaleric acid

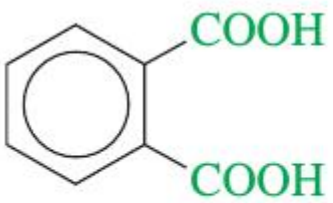


3-methylbutanoic acid
isovaleric acid

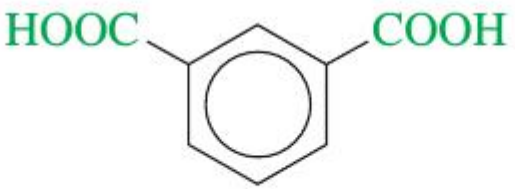
Néhány kétértékű karbonsav (dikarbonsav)

TABLE 20-2 Names and Physical Properties of Dicarboxylic Acids

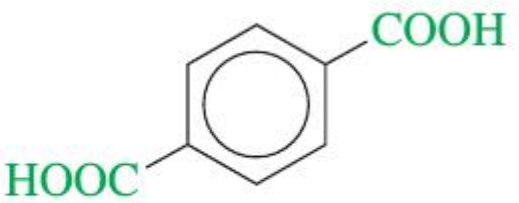
IUPAC Name	Common Name	Formula	mp (°C)	Solubility (g/100 g H_2O)
ethanedioic	oxalic	HOOC—COOH	189	14
propanedioic	malonic	$HOOCCH_2COOH$	136	74
butanedioic	succinic	$HOOC(CH_2)_2COOH$	185	8
pentanedioic	glutaric	$HOOC(CH_2)_3COOH$	98	64
hexanedioic	adipic	$HOOC(CH_2)_4COOH$	151	2
heptanedioic	pimelic	$HOOC(CH_2)_5COOH$	106	5
cis-but-2-enedioic	maleic	*cis*-HOOCCH=CHCOOH	130.5	79
trans-but-2-enedioic	fumaric	*trans*-HOOCCH=CHCOOH	302	0.7
benzene-1,2-dicarboxylic	phthalic	$1,2\text{-}C_6H_4(COOH)_2$	231	0.7
benzene-1,3-dicarboxylic	isophthalic	$1,3\text{-}C_6H_4(COOH)_2$	348	
benzene-1,4-dicarboxylic	terephthalic	$1,4\text{-}C_6H_4(COOH)_2$	300 sublimes	0.002



o-phthalic acid
phthalic acid

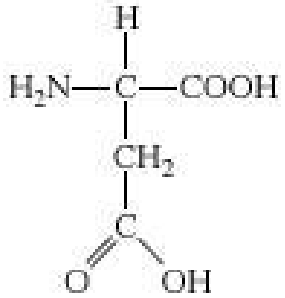


m-phthalic acid
isophthalic acid

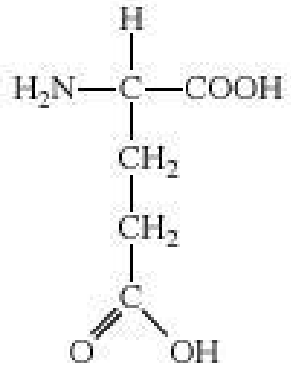


p-phthalic acid
terephthalic acid

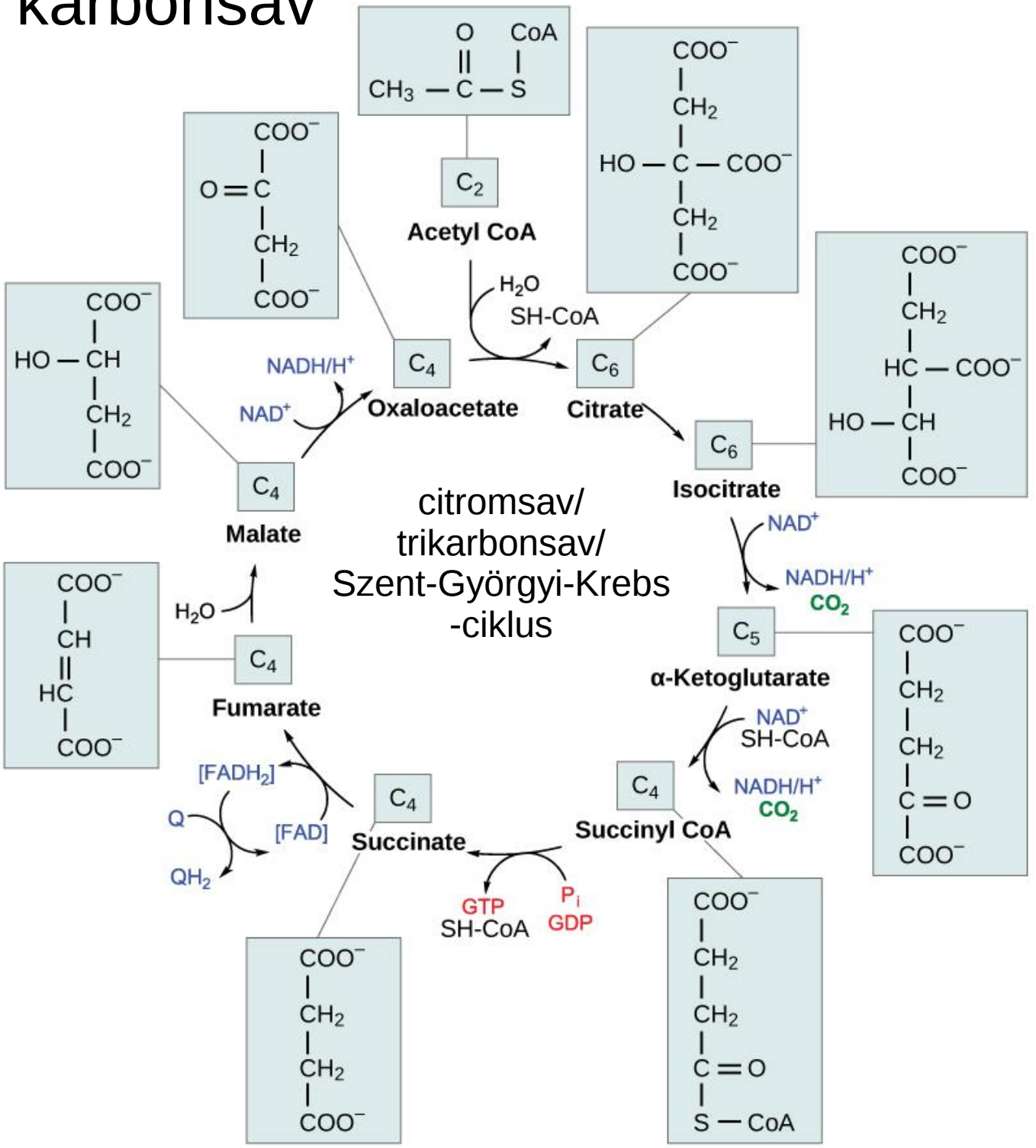
Néhány fontosabb karbonsav



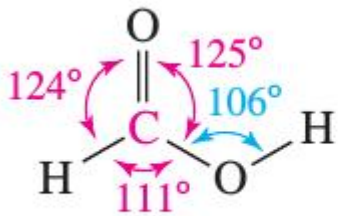
aszparaginsav
(Asp, D)



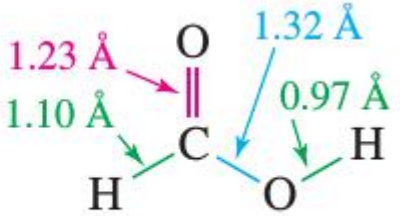
glutaminsav
(Glu, E)



A karboxilcsoport és a karbonsavak fizikai tulajdonságai

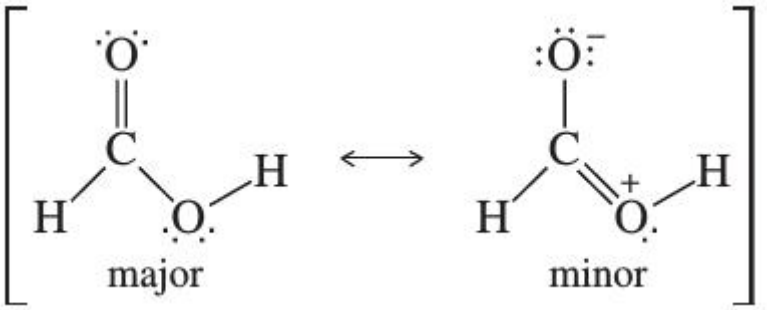


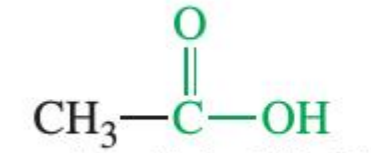
bond angles



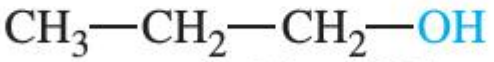
bond lengths

A karboxilcsoport határszerkezetei (példa: hangyasav)

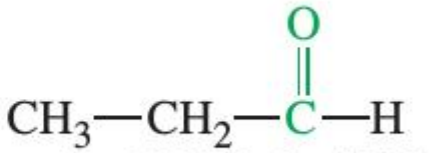




acetic acid, bp 118 °C

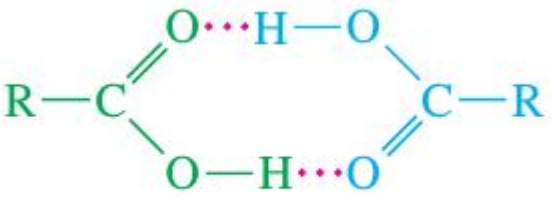


propan-1-ol, bp 97 °C



propionaldehyde, bp 49 °C

A karbonsavak magas forráspontja a karboxilcsoportok közötti hidrogénkötések létrejöttével magyarázható



hydrogen-bonded acid dimer

Karbonsavak savassága (aciditása)

		K_a (at 25 °C)	pK_a
HCOOH	formic acid	1.77×10^{-4}	3.75
CH_3COOH	acetic acid	1.76×10^{-5}	4.74
CH_3CH_2 COOH	propionic acid	1.34×10^{-5}	4.87
$CH_3(CH_2)_2COOH$	butyric acid	1.54×10^{-5}	4.82
$CH_3(CH_2)_3COOH$	pentanoic acid	1.52×10^{-5}	4.81
$CH_3(CH_2)_4COOH$	hexanoic acid	1.31×10^{-5}	4.88
$CH_3(CH_2)_6COOH$	octanoic acid	1.28×10^{-5}	4.89
$CH_3(CH_2)_8COOH$	decanoic acid	1.43×10^{-5}	4.84
C_6H_5 COOH	benzoic acid	6.46×10^{-5}	4.19
p-$CH_3C_6H_4COOH$	*p*-toluic acid	4.33×10^{-5}	4.36
p-ClC_6H_4COOH	*p*-chlorobenzoic acid	1.04×10^{-4}	3.98
p-$NO_2C_6H_4COOH$	*p*-nitrobenzoic acid	3.93×10^{-4}	3.41

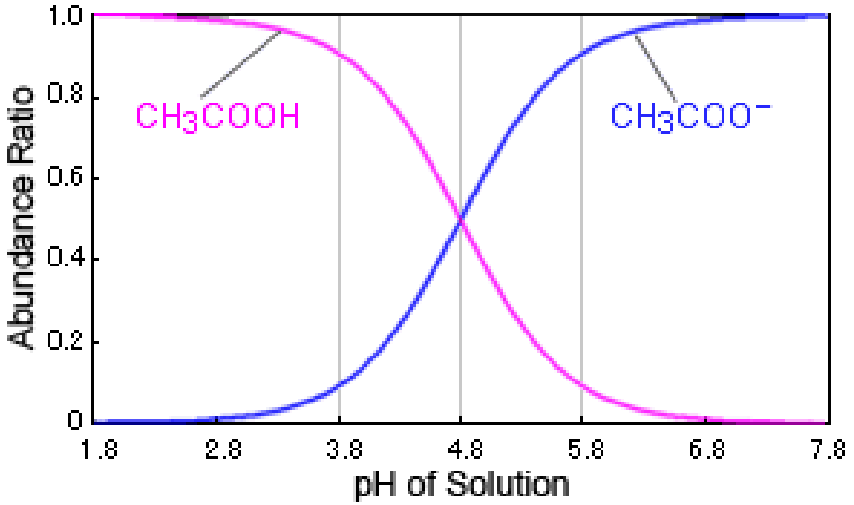
karboxilát ion

Az ásványi savaknál gyengébb, de a szerves vegyületek között viszonylag erős savaknak számítanak.

$$K_a = \frac{[R—CO_2^-][H_3O^+]}{[R—CO_2H]}$$

$$pK_a = -\log_{10} K_a$$

Karbonsavak savassága (aciditása)



A pK_a a savi disszociációs állandó negatív logaritmusa, adott csoportra jellemző érték.

A pK_a értelmezése: az a pH, ahol az adott csoport disszociációja 50%-os
Az ecetsav példáján:
$[CH_3COOH] = [CH_3COO^-]$

Kisebb pK_a erősebb savat jelent.
A pK_a-nál alacsonyabb pH-n a csoport protonált, annál magasabb pH-n a csoport deprotonált formában van főként jelen.

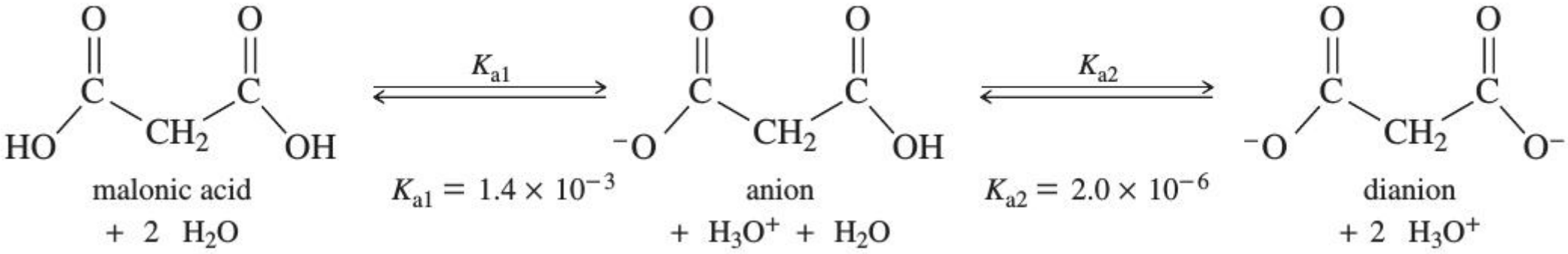
karboxilát ion

$$K_a = \frac{[R—CO_2^-][H_3O^+]}{[R—CO_2H]}$$

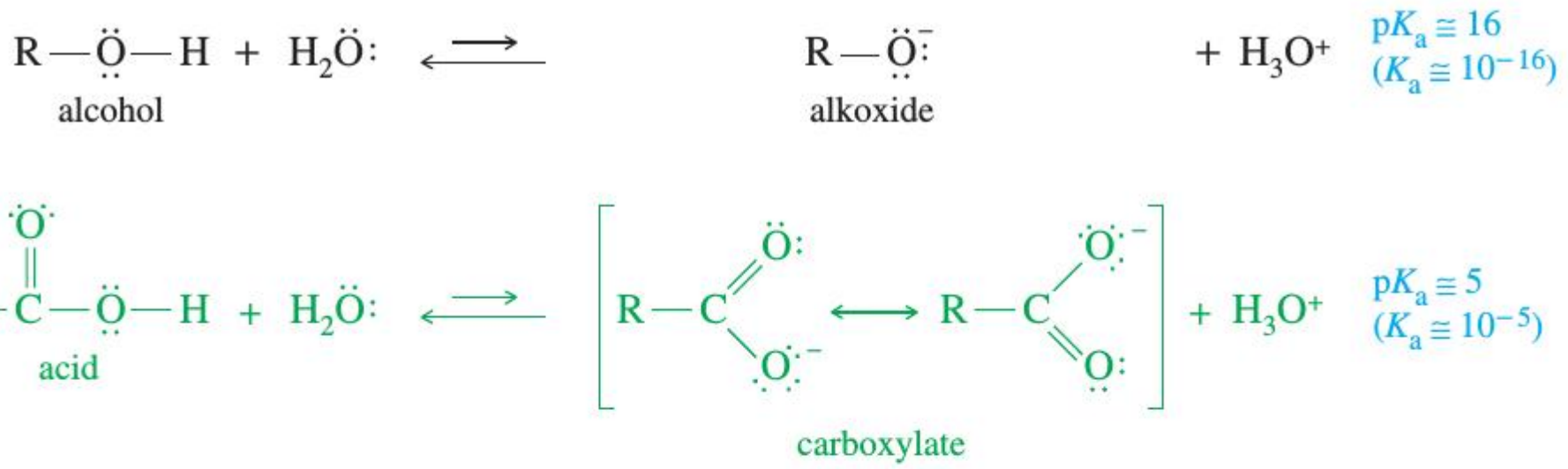
$$pK_a = -\log_{10} K_a$$

Dikarbonsavak savassága (aciditása)

		K_{a1}	pK_{a1}	K_{a2}	pK_{a2}
HOOC—COOH	oxalic	5.4×10^{-2}	1.27	5.2×10^{-5}	4.28
$HOOCCH_2COOH$	malonic	1.4×10^{-3}	2.85	2.0×10^{-6}	5.70
$HOOC(CH_2)_2COOH$	succinic	6.4×10^{-5}	4.19	2.3×10^{-6}	5.64
$HOOC(CH_2)_3COOH$	glutaric	4.5×10^{-5}	4.35	3.8×10^{-6}	5.42
$HOOC(CH_2)_4COOH$	adipic	3.7×10^{-5}	4.43	3.9×10^{-6}	5.41
cis-HOOCCH=CHCOOH	maleic	1.0×10^{-2}	2.00	5.5×10^{-7}	6.26
trans-HOOCCH=CHCOOH	fumaric	9.6×10^{-4}	3.02	4.1×10^{-5}	4.39
$1,2\text{-}C_6H_4(COOH)_2$	phthalic	1.1×10^{-3}	2.96	4.0×10^{-6}	5.40
$1,3\text{-}C_6H_4(COOH)_2$	isophthalic	2.4×10^{-4}	3.62	2.5×10^{-5}	4.60
$1,4\text{-}C_6H_4(COOH)_2$	terephthalic	2.9×10^{-4}	3.54	3.5×10^{-5}	4.46

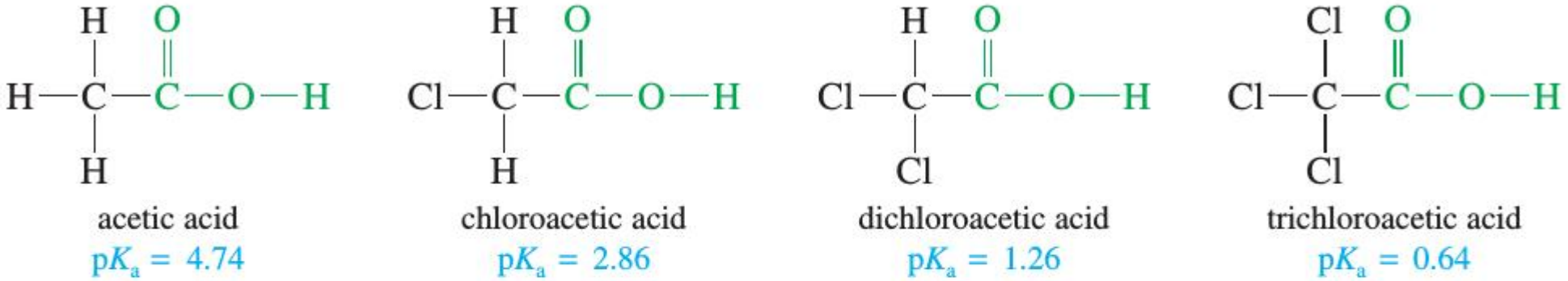


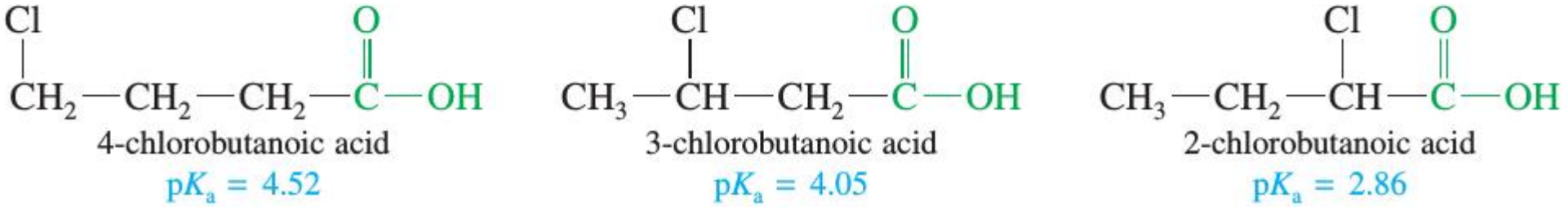
Alkoholok és karbonsavak aciditása



A karboxilát esetében a negatív töltés eloszlik a két oxigénatom között, a delokalizáció növeli a deprotonált forma stabilitását.

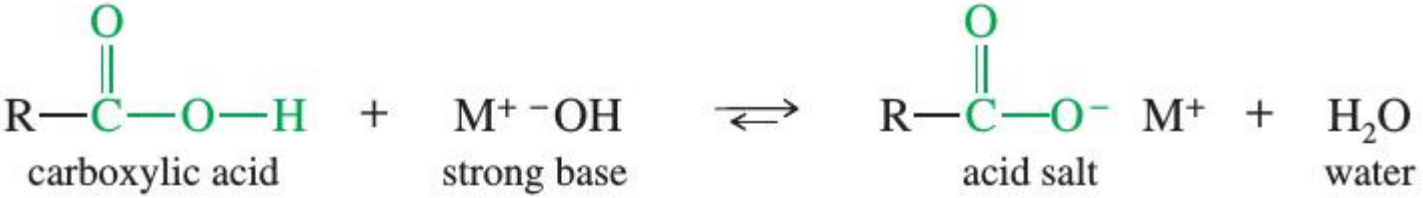
Halogénezett karbonsavak aciditása





A halogénatomok elektronszívó hatása stabilizálja a karboxilát iont
Minél több halogénatom ill. a karboxilcsoporthoz minél közelebb kapcsolódik, annál nagyobb a hatás.

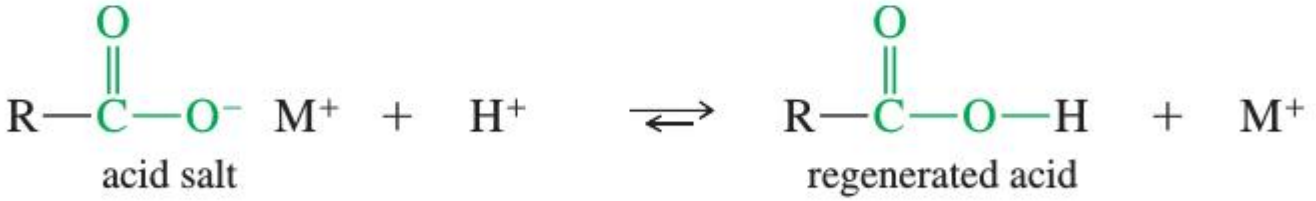
Karbonsavak sói



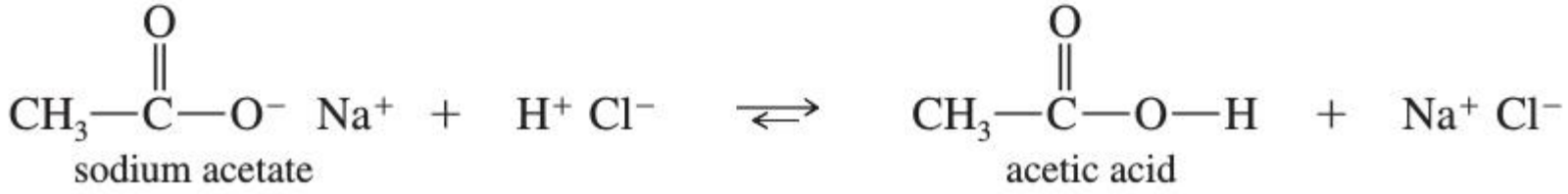
For example, sodium hydroxide deprotonates acetic acid to form sodium acetate, the sodium salt of acetic acid.

ecetsav nátrium-hidroxid nátrium-acetát

Egy erős bázis, mint a nátrum-hidroxid, deprotonálja az ecetsavat,
és nátrium-acetát keletkezik



Erős ásványi savval a karbonsavak felszabadíthatóak sóikból.



Kitekintés: a vízkő kémiája

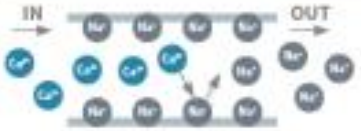
THE CHEMISTRY OF LIMESCALE

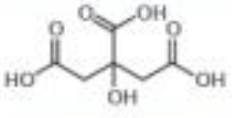
Limescale can clog up your kitchen appliances, and build up on your bathroom surfaces. What actually causes this build up? Here's a quick look at the chemistry behind limescale formation, chemicals that can help prevent it, and others that help to remove it.

WATER HARDNESS

'Hard water' is water which contains a large amount of mineral ions, most commonly calcium and magnesium ions. Permanent hard water is mainly due to dissolved calcium and magnesium sulfates. Temporary hard water is mainly due to dissolved calcium bicarbonate. Temporary hardness can be removed by boiling the water, but permanent hardness cannot.

WATER SOFTENERS





Appliances such as dishwashers can soften water by passing it through an ion exchange resin. This exchanges scale-causing metal ions in the water for sodium ions. Compounds such as citric acid and sodium sesquicarbonate can be used to soften laundry water.

LIMESCALE & SOAP SCUM

$$Ca^{2+}_{(aq)} + 2HCO_3^-{}_{(aq)} \rightleftharpoons CaCO_{3(s)} + CO_{2(aq)} + H_2O_{(l)}$$

Calcium bicarbonate can decompose when heated to form insoluble calcium carbonate – known in this context as limescale – along with water and carbon dioxide. This process removes the temporary hardness from water that the calcium bicarbonate causes.

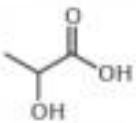
$$2(C_{18}H_{35}O_2)^-_{(aq)} + Mg^{2+}_{(aq)} \longrightarrow Mg(C_{18}H_{35}O_2)_{2(s)}$$

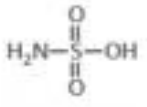
Calcium and magnesium ions in the water can also react with the fatty acids found in soaps to produce insoluble compounds that form a soap scum on bathroom surfaces. The example shown above is that of stearate ions reacting to produce magnesium stearate.

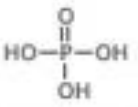
Limescale consists mainly of calcium carbonate. It can also contain small amounts of the following compounds, depending on water composition:

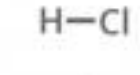
calcium sulfate
barium sulfate
magnesium hydroxide
calcium phosphate
zinc phosphate
iron hydroxides

REMOVING LIMESCALE







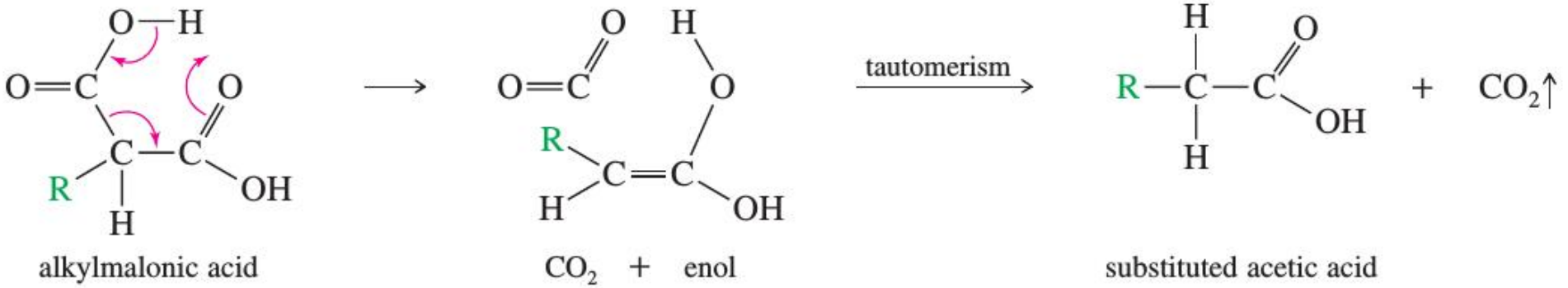


Once limescale has been formed, it can be removed from appliances or surfaces by reacting it with an acid. A variety of acids can be used, all of which react with the calcium carbonate to produce a soluble calcium salt, along with carbon dioxide and water as side products.

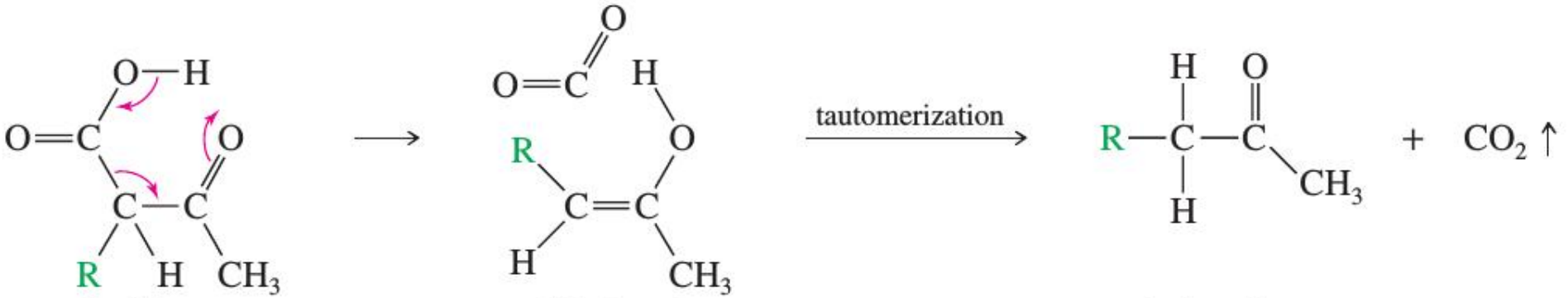
Dekarboxilációs reakciók

(Többek között) a β-helyzetben karbonil csoportot hordozó karbonsavak hajlamosak rá.

Figyeljük meg az enol forma megjelenését! Mire emlékeztet a reakció?

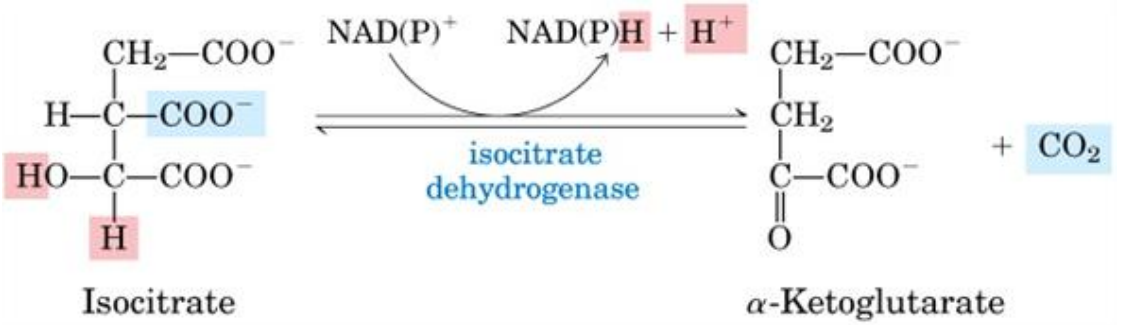


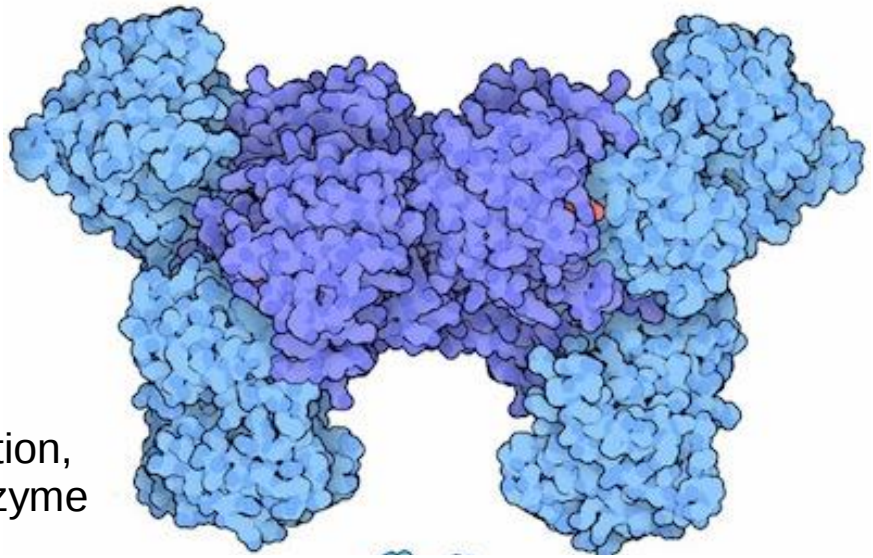
alkylmalonic acid — CO_2 + enol — substituted acetic acid



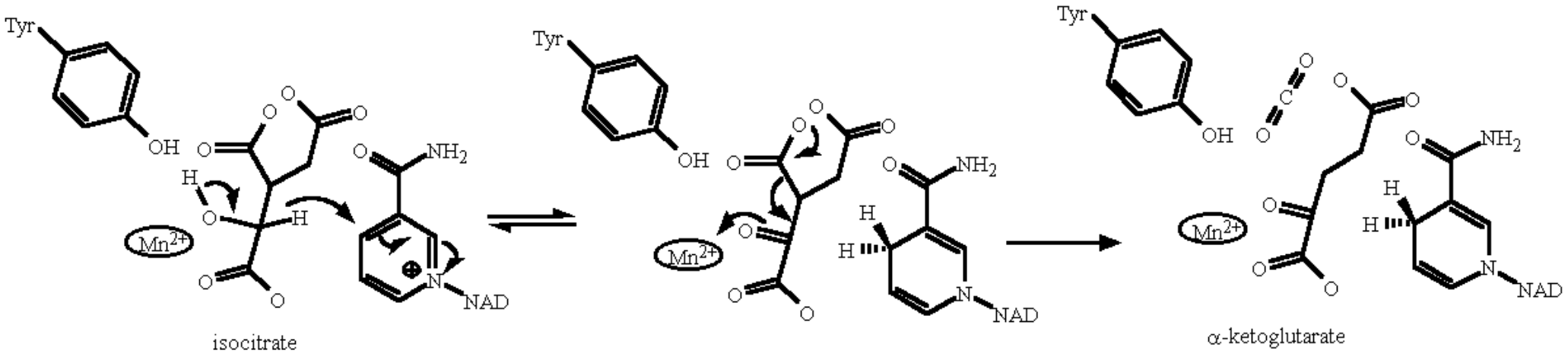
the β-keto acid — CO_2 + enol — a substituted acetone

Kitekintés: az izocitrát dehidrogenáz enzim





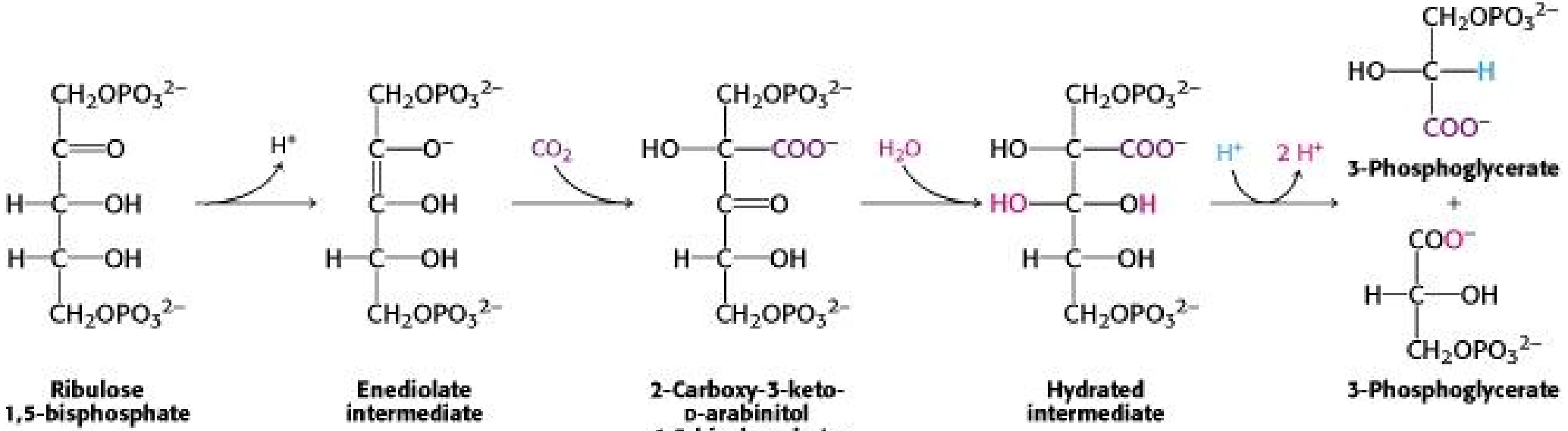
Four catalytic chains (colored turquoise here) perform the reaction, and four regulatory chains (colored dark blue here) turn the enzyme on and off based on the levels of ATP and ADP in our cells

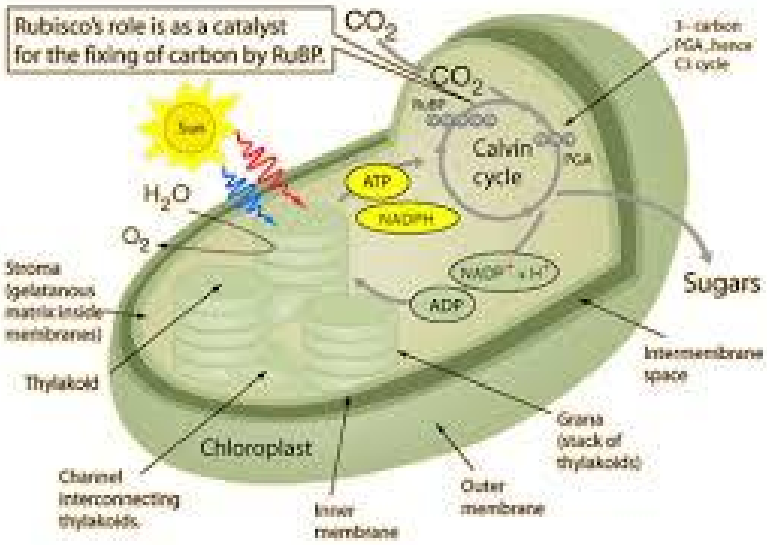


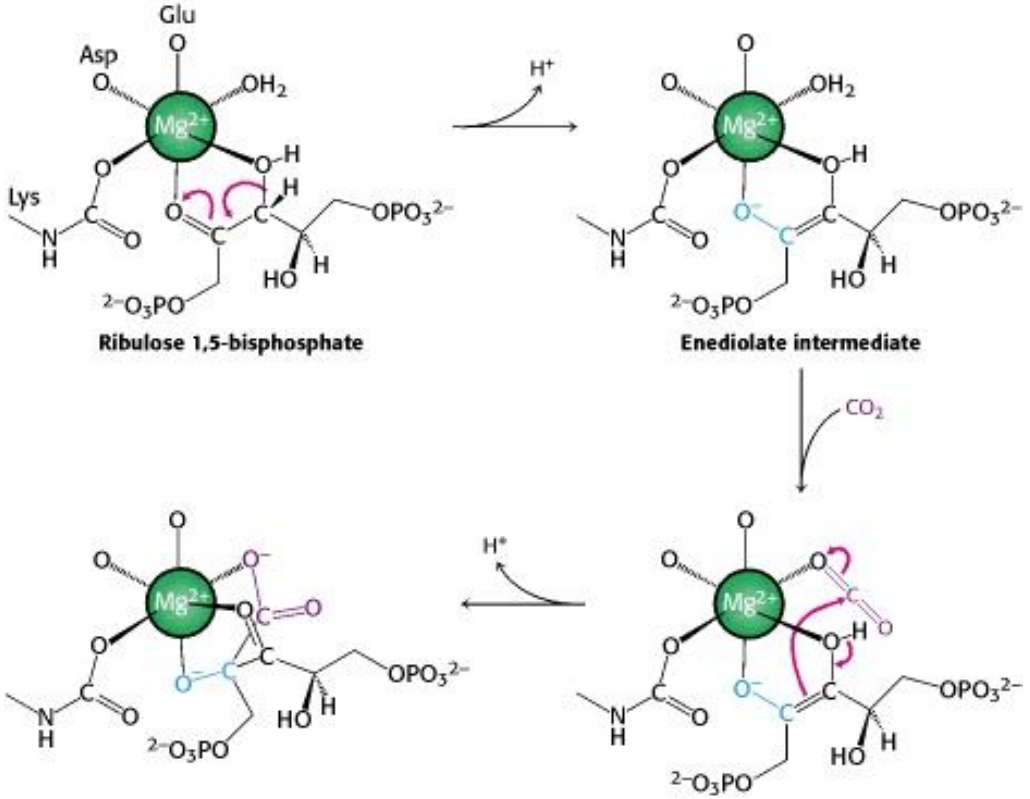
A citromsav-ciklus első dekarboxilezését katalizálja. Figyeljük meg a(z eltávolított karobxilcsoporthoz képest) β-ketosav kialakítását (oxidációs lépés) a dekarboxiláció előtt! A dekarboxiláció mechanizmusa hasonló az előző oldalon bemutatotthoz.

Kitekintés: a RuBisCO enzim

Ribulóz 1,5-biszfoszfát karboxiláz/oxigenáz: a növények CO_2 fixálásáért felelős enzim

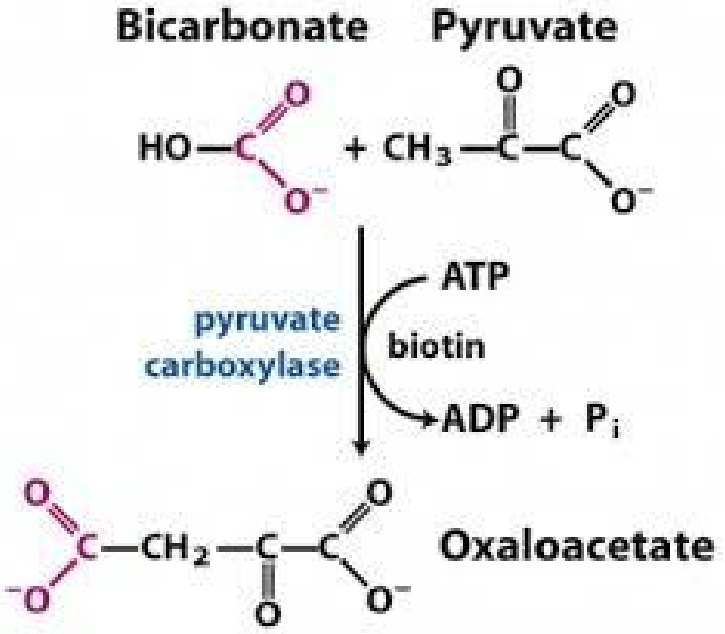




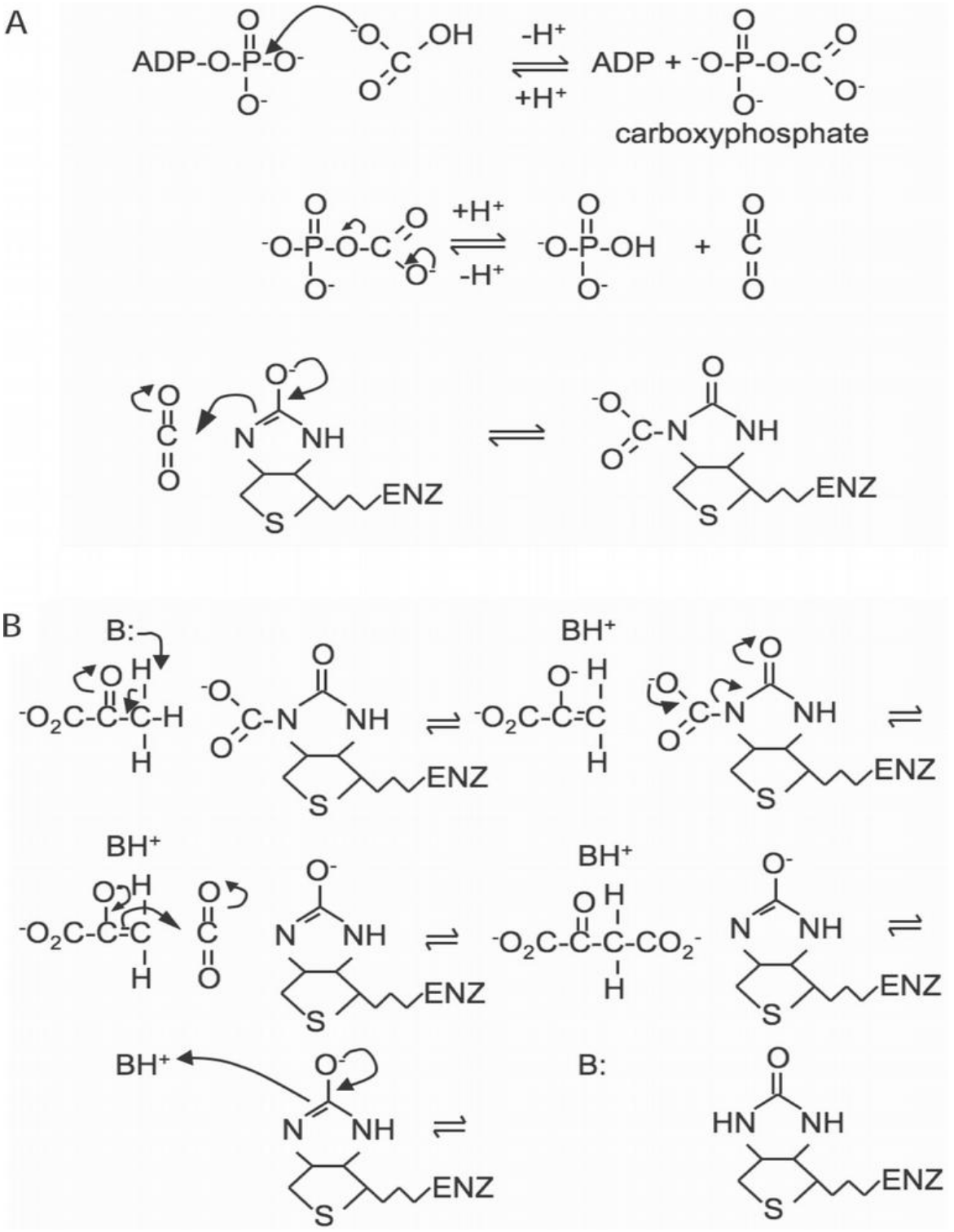


Az aktív centrumban lévő magnéziumion egyik koordinálója egy CO_2 molekulával módosított lizin oldallánc. A cukorhoz kapcsolt CO_2 ettől különbözik!

Kitekintés: a piruvát karboxiláz enzim mechanizmusa



Az “oxálecetsav-készlet feltöltésének” fontos reakciója



Sarawut Jitrapakdee et al. Biochem. J. 2008;413:369-387

Kitekintés: karboxiláció-dekarboxikláció a zsírsavak bioszintézisében

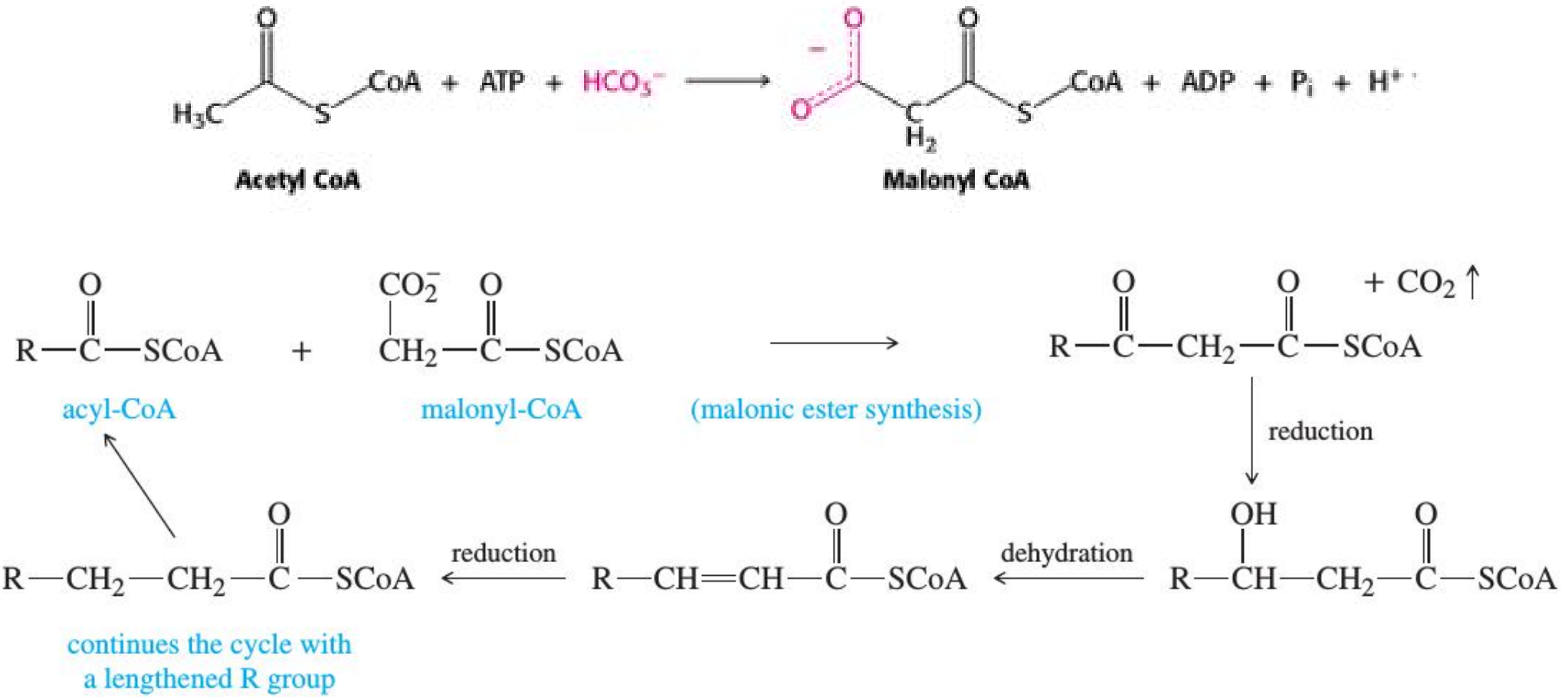


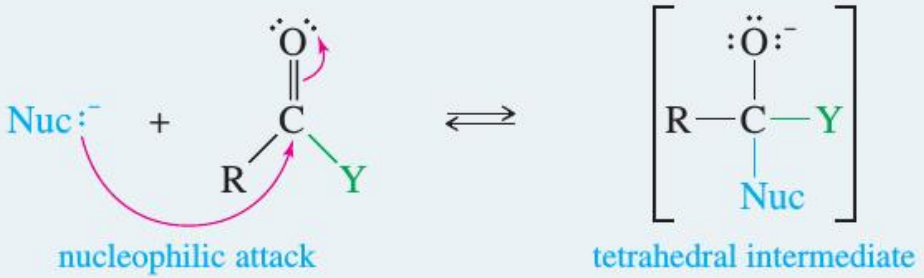
FIGURE 22-3
Fatty acid biosynthesis. Activated as its coenzyme A thioester, the growing fatty acid (acyl-CoA) acylates malonyl-CoA in a malonic ester synthesis. Two carbon atoms are added, with the third lost as CO_2. Enzymatic reduction, dehydration, and further reduction gives a fatty acid that has been lengthened by two carbon atoms.

Nukleofil acil szubsztitúció

Karbonsavak és származékaik alapvető reakciója, ilyen reakciók segítségével alakíthatóak egymásba az egyes karbonsavszármazékok.
Emlékezzünk, hogy a karbonil szénatom elektronhiányos!
DE: a ketonokkal és aldehidekkel ellentétben a karbonsavakra és származékaikra nem az addíció, hanem a szubsztitúció a jellemző reakció!

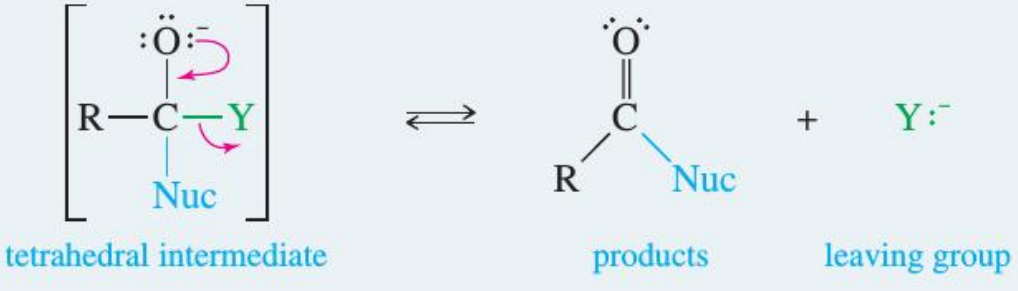
Addíciós-eliminációs mechanizmus:

Step 1: Addition of the nucleophile gives a tetrahedral intermediate.



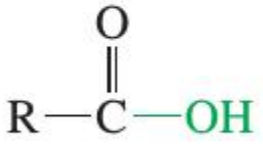
tetraéderes intermedier

Step 2: Elimination of the leaving group regenerates the carbonyl group.



távozó csoport

Fontosabb karbonsavszármazékok áttekintése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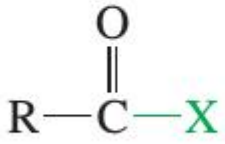
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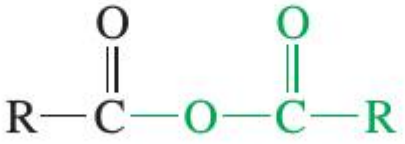
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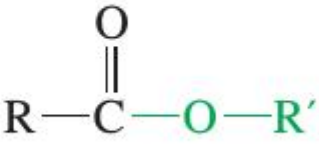
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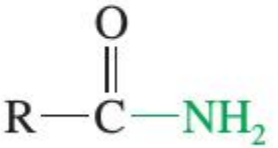
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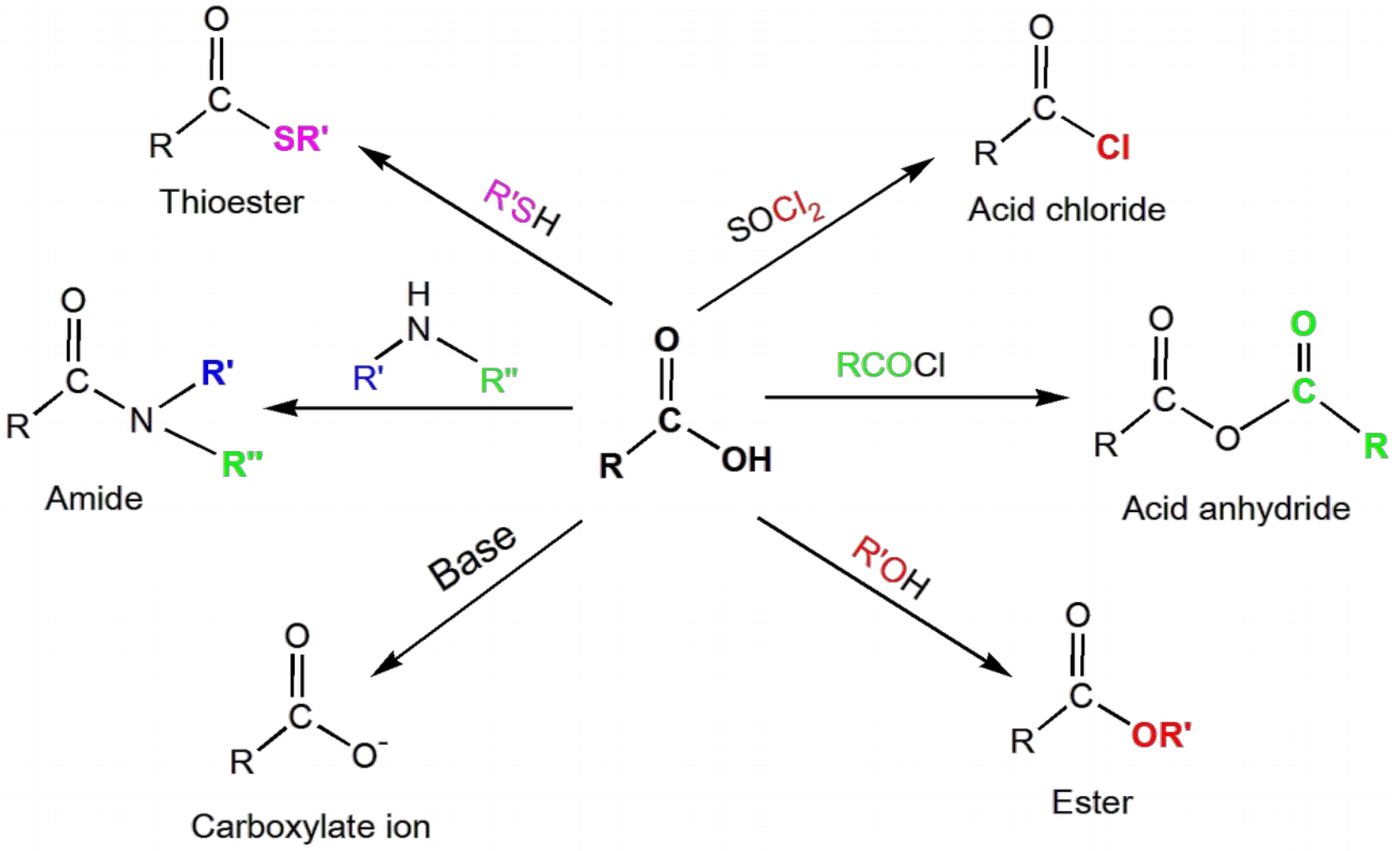
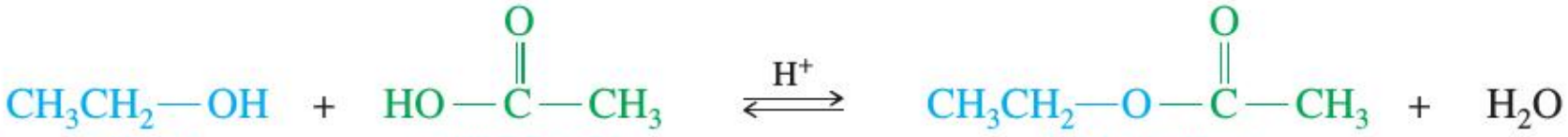
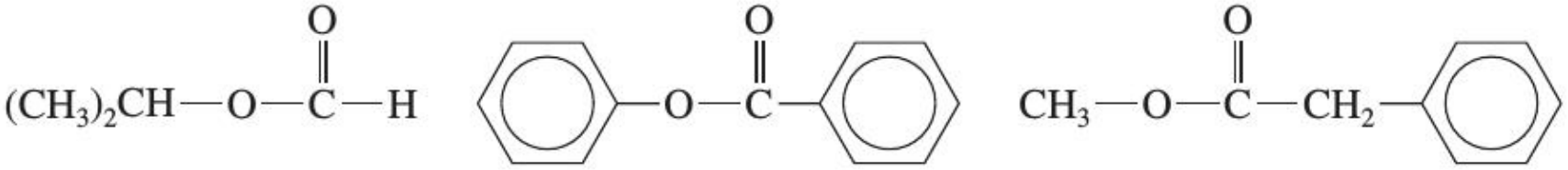
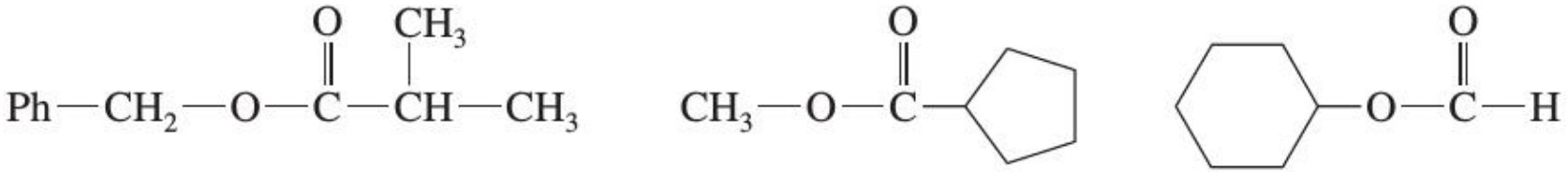
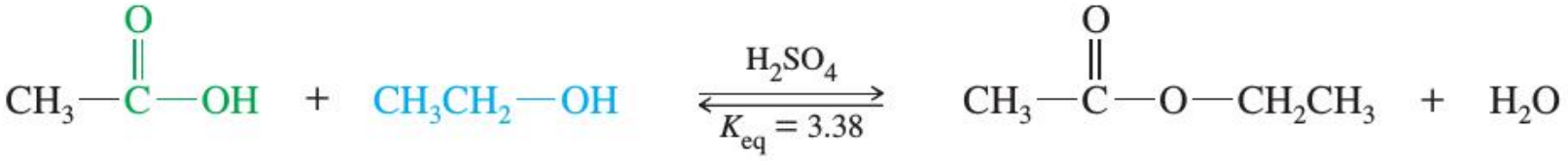


Észterek képződése, egyszerű példák

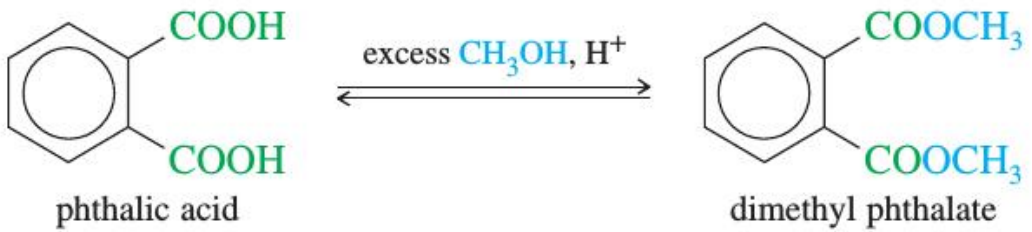








Név: az alkohol nevének “töve” + a savmaradék neve



Észterek képződése: mechanizmus

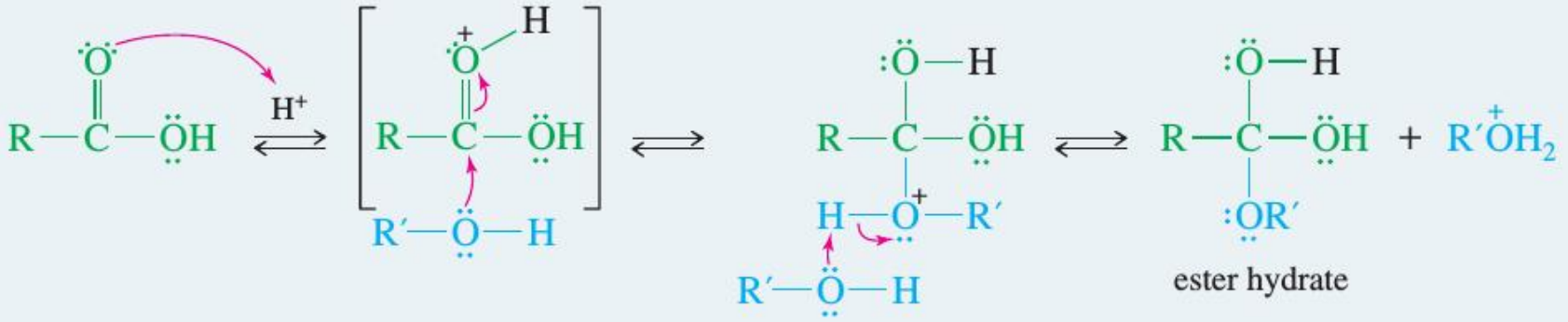
A savkatalizált nukleofil acil szubsztitúció példája Emlékezzünk, hogy az első protonálási lépés növeli a karbonil szén érzékenységét nukleofil támadásokra.

Part 1: *Acid-catalyzed addition of the alcohol to the carbonyl group.*

Protonation activates the carbonyl.

The alcohol adds.

Deprotonation completes the reaction.



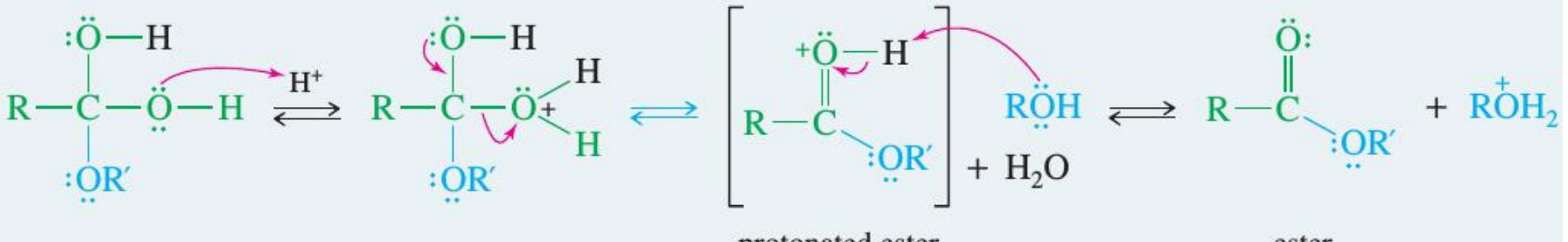
(Species in brackets are resonance-stabilized.)

Part 2: *Acid-catalyzed dehydration.*

Protonation prepares the OH group to leave.

Water leaves.

Deprotonation completes the reaction.



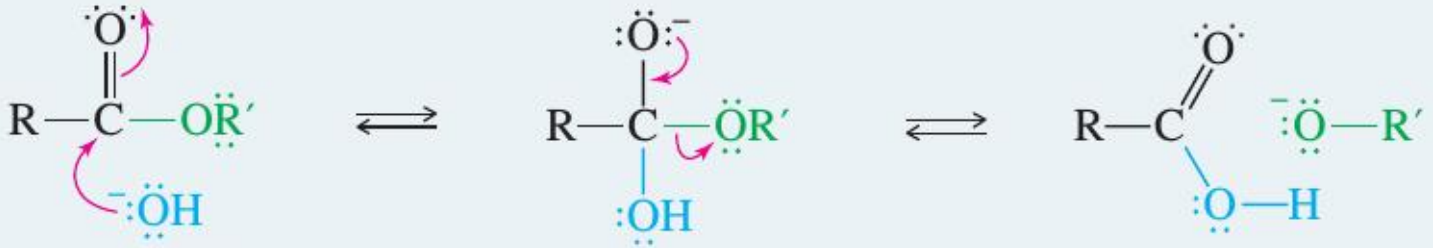
Észterek hidrolízise: mechanizmus

Ez is nukleofil acil szubsztitúció, de bázikus közegben (a hidroxidion a nukleofil).

MECHANISM 20-1 Nucleophilic Acyl Substitution in the Basic Hydrolysis of an Ester

Step 1: Hydroxide ion adds to the carbonyl group, forming a tetrahedral intermediate.

Step 2: An alkoxide ion leaves, regenerating the C=O double bond.



ester + $^-$OH

tetrahedral intermediate

acid + alkoxide

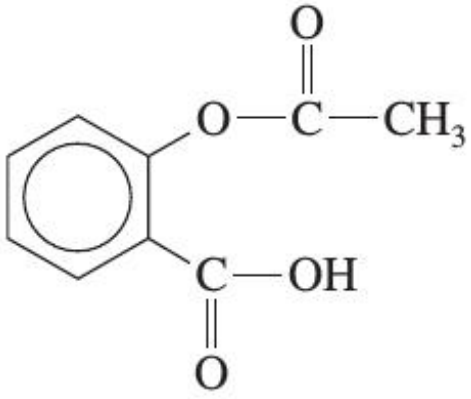
Step 3: A fast, exothermic proton transfer drives the reaction to completion.

acid + alkoxide

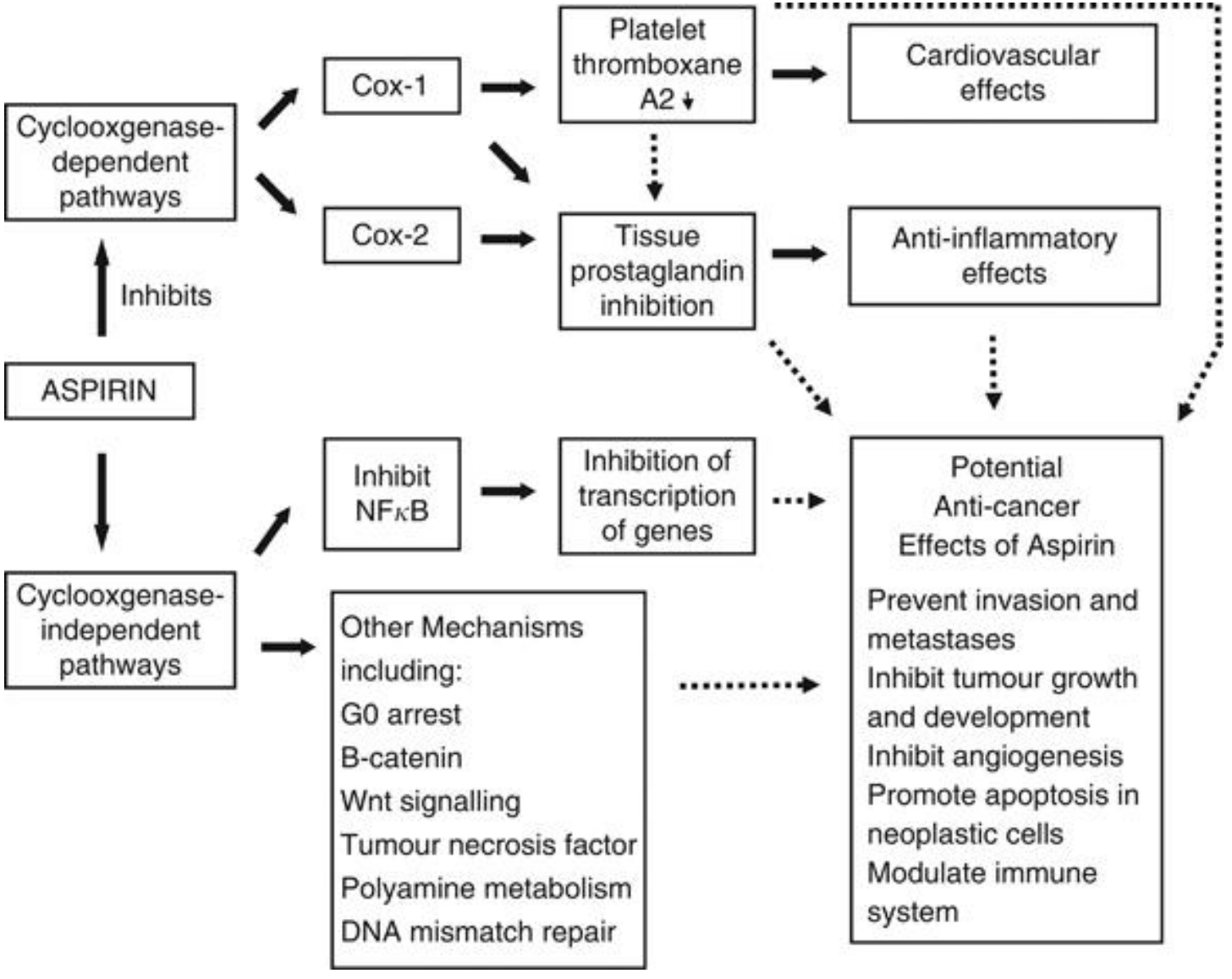
carboxylate + alcohol

Kitekintés: az aszpirin

Felix Hoffman, working at the Bayer company in Germany, made the acetylated form of salicylic acid in 1897. This drug was named "Aspirin" and became the most widely used medicine of all time. In 1971, Vane discovered the mechanism by which aspirin exerts its anti-inflammatory, analgesic and antipyretic actions. He proved that aspirin and other non-steroid anti-inflammatory drugs (NSAIDs) inhibit the activity of the enzyme now called cyclooxygenase (COX) which leads to the formation of prostaglandins (PGs) that cause inflammation, swelling, pain and fever.



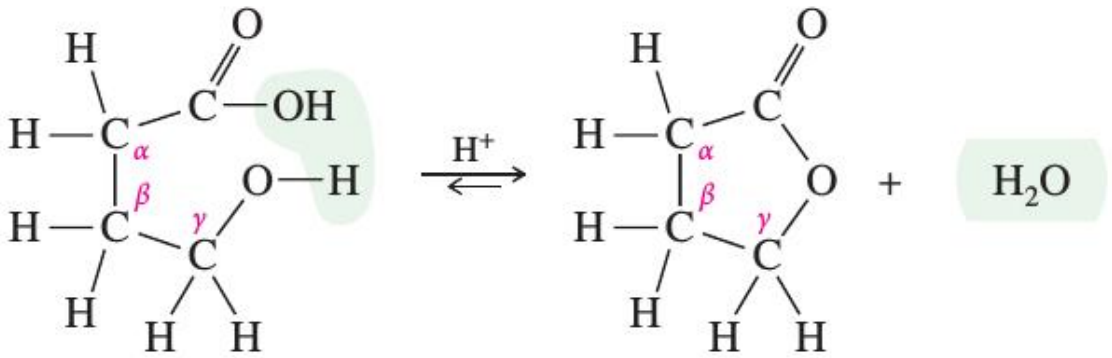
acetylsalicylic acid
(aspirin)



Gyűrűs észterek: laktonok

Lactones Cyclic esters are called **lactones.** A lactone is formed from an open-chain hydroxy acid in which the hydroxyl group has reacted with the acid group to form an ester.

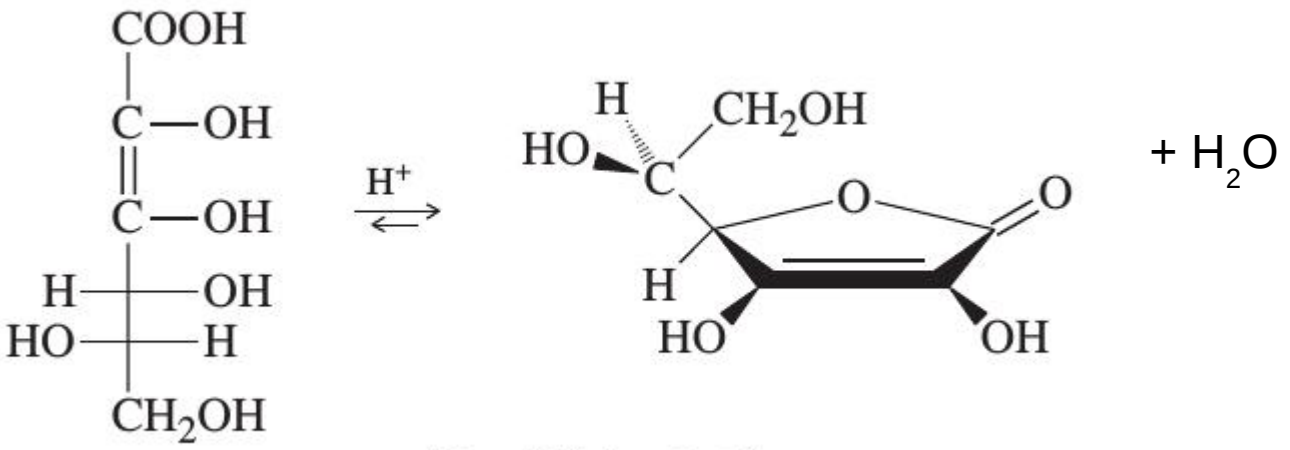
A karboxil- és a hidroxilcsoport ugynazon molekulában található



IUPAC name: 4-hydroxybutanoic acid — 4-hydroxybutanoic acid lactone
common name: γ-hydroxybutyric acid — γ-butyrolactone

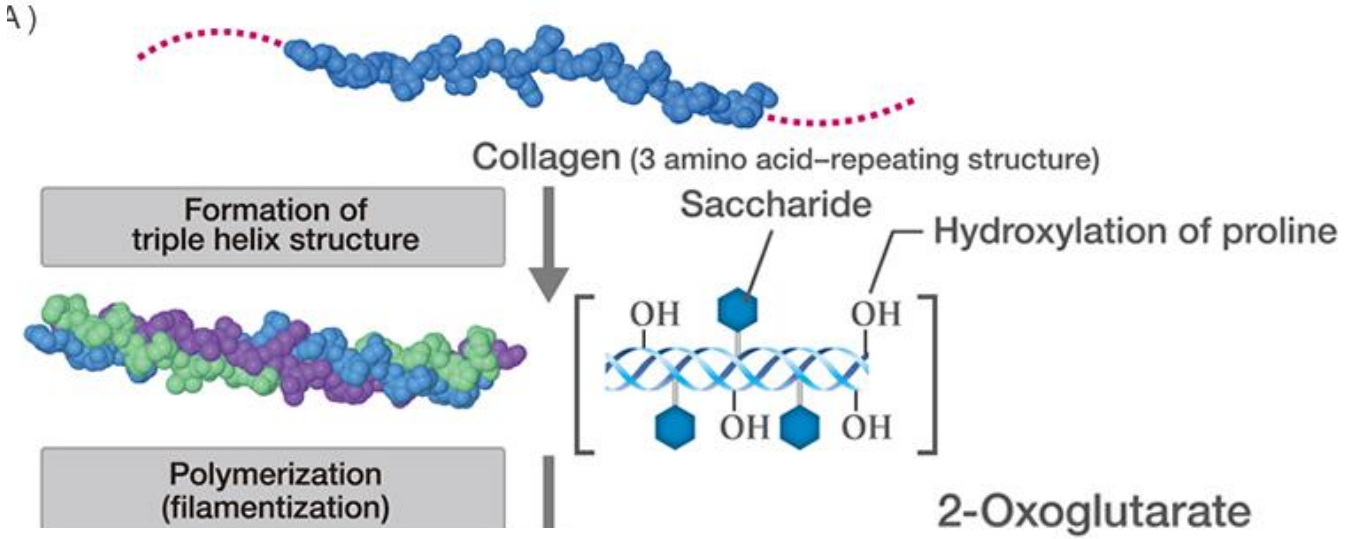
Az aszkorbinsav

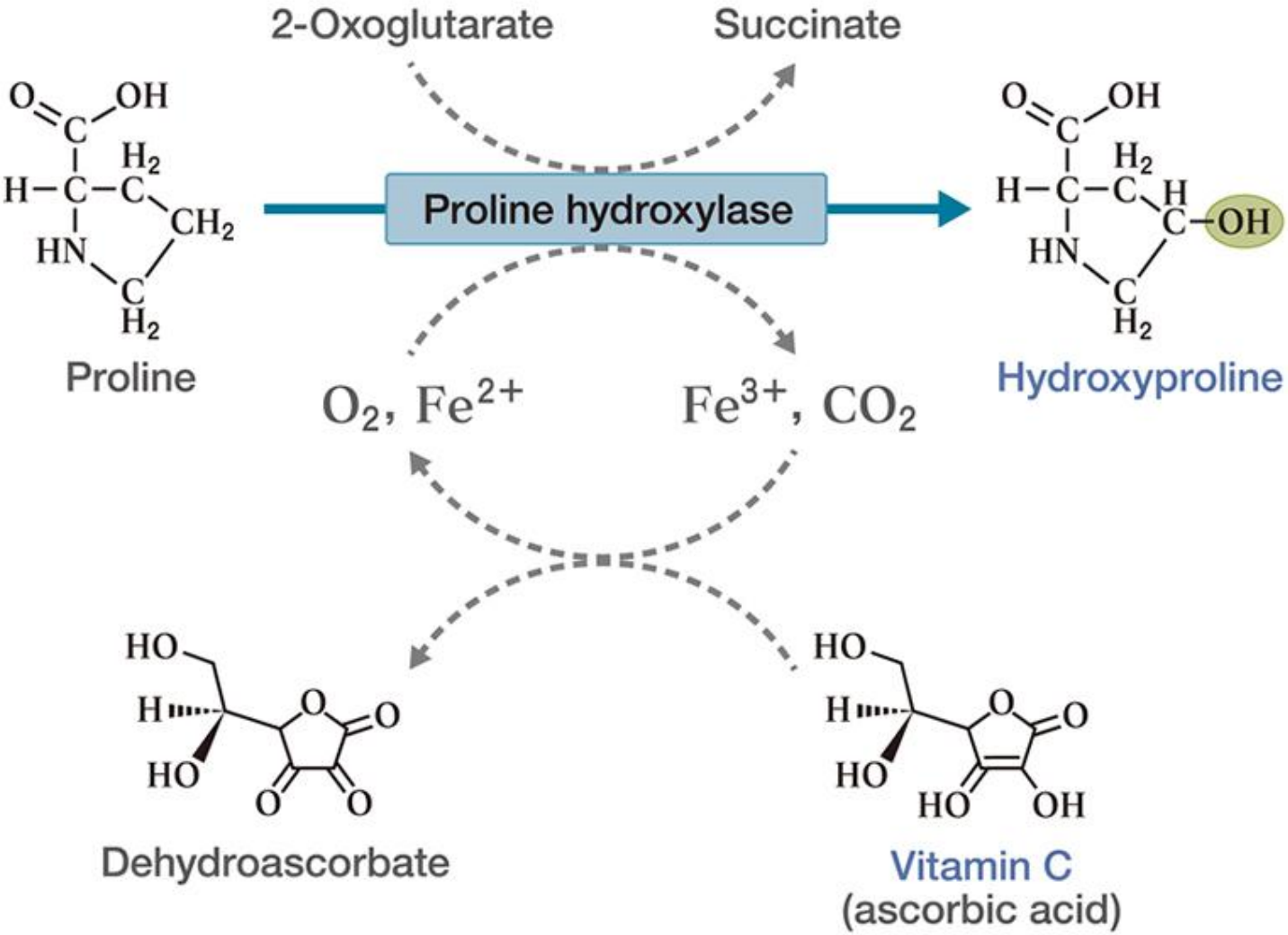
Figyeljük meg, hogy (a szénhidrátokkal ellentétben) a nyílt láncú és a gyűrűs forma nem izomer, hiszen **vízkilépés** történik az észterkötés kialakulásakor.



L-ascorbic acid (vitamin C)

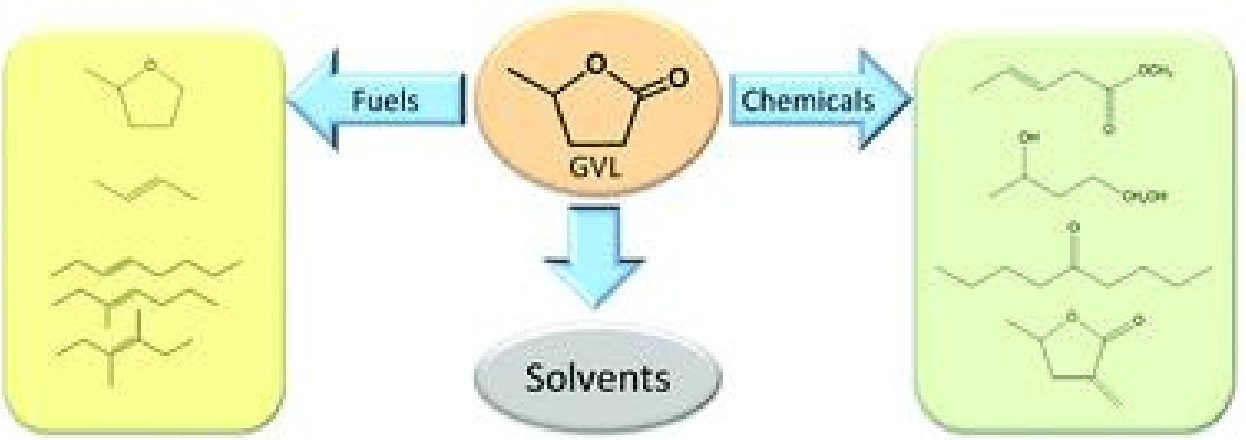
Kitekintés: skorbut és a C-vitamin

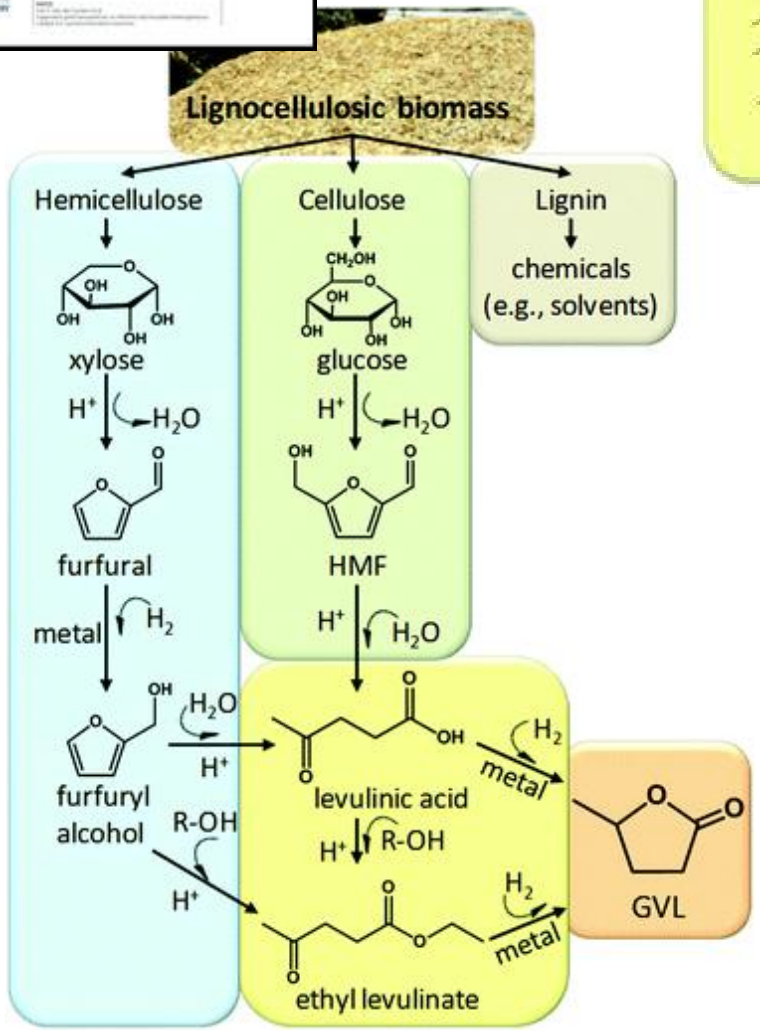




A C-vitamin elengedhetetlen a kollagén egyes prolin aminosavaira hidroxilcsoportot szintetizáló enzim regenerálásához.
A hidroxiprolin hiányában a kötőszöveti rostok elvesztik mechanikai tartásukat, a fogak kihullanak, az ízületekben belső vérzések alakulnak ki stb.

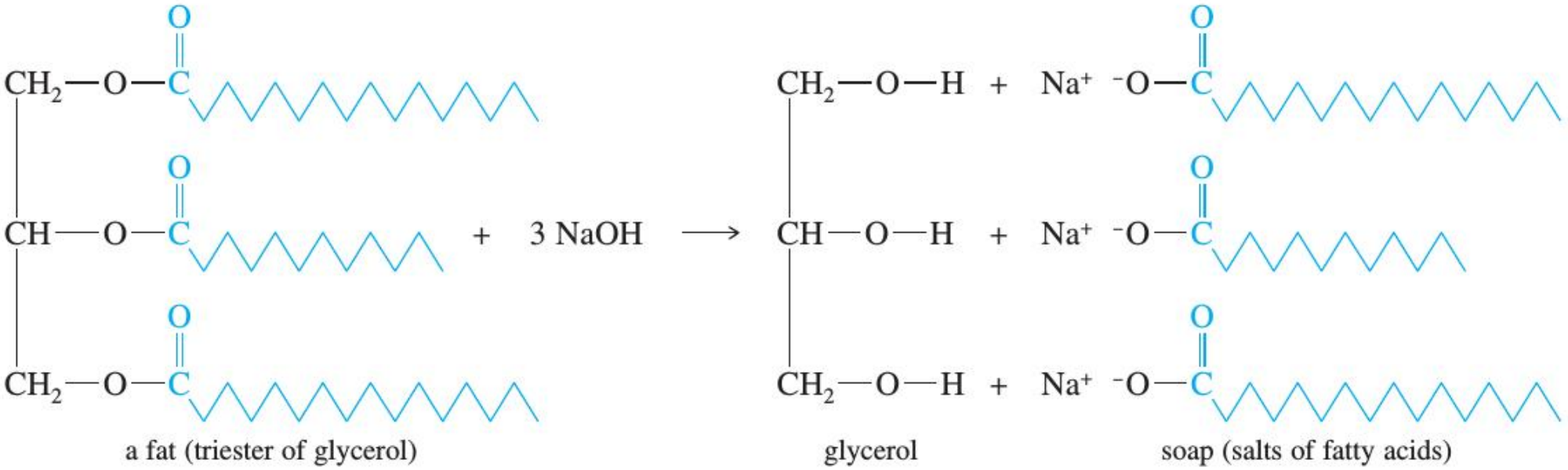
Kitekintés: a γ-valerolakton mint “zöld alapanyag”





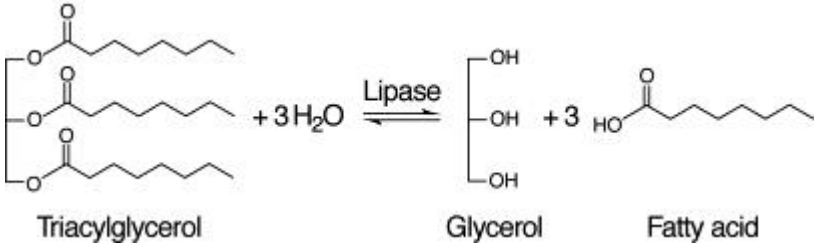
We propose that γ-valerolactone (GVL), a naturally occurring chemical in fruits and a frequently used food additive, exhibits the most important characteristics of an ideal sustainable liquid, which could be used for the production of both energy and carbon-based consumer products. GVL is renewable, easy and safe to store and move globally in large quantities, has low melting (−31 °C), high boiling (207 °C) and open cup flash (96 °C) points, a definitive but acceptable smell for easy recognition of leaks and spills, and is miscible with water, assisting biodegradation.

Észterek hidrolízise: zsírok elszappanosítása

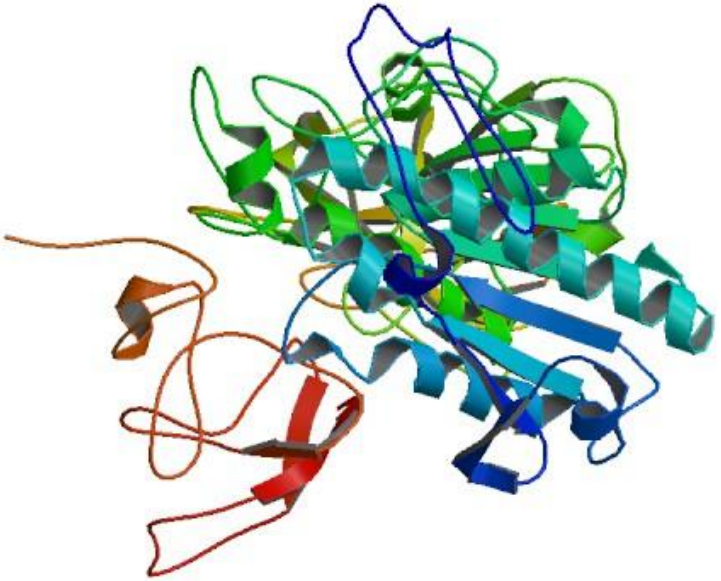


Hosszú szénláncú zsírsavak sói keletkeznek, a szappanokról lásd a lipides előadást.

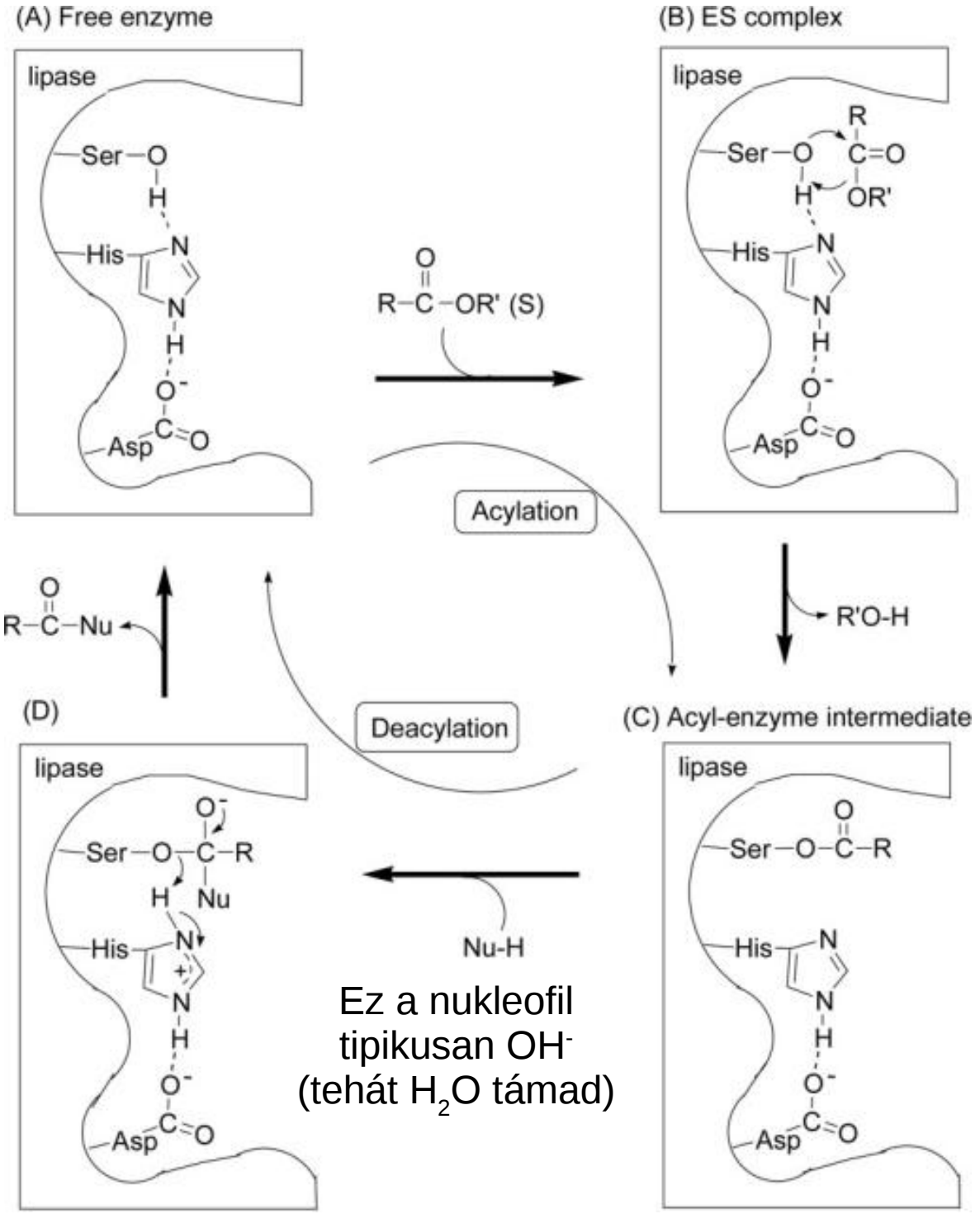
Kitekintés: lipázok mechanizmusa



Két nukleofil acil szubsztitúciós lépés



Lipáz és kolipáz (a piros alegység balra lent, a lipidrészecskék felszínéhez való asszociációt segíti) fehérje szerkezete



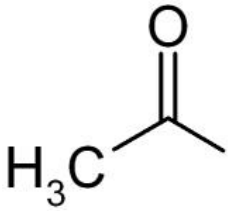
Ez a nukleofil tipikusan OH^- (tehát H_2O támad)

Karbonsavakból származtatott csoportok nevei

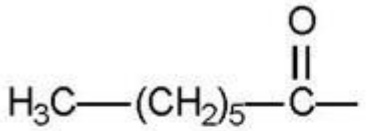
A karboxikcsoportból a hidrogén elhagyásával kapott csoport a savmaradék, az OH elhagyásával kapott csoport az acilcsoport.

acilcsoport

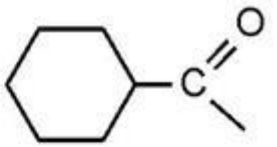
lásd:
nuklefil acil szubsztitúció,
acilezés,
acil-koenzim-A



acetilcsoport: az ecetsavból származtatható acilcsoport



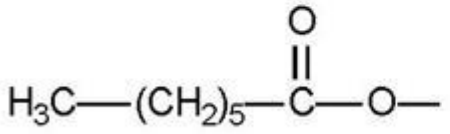
heptanoil



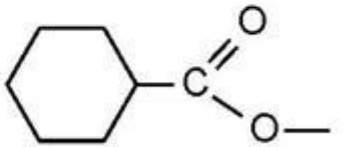
ciklohexánkarbonil

savmaradék

lásd:
észterek nevei



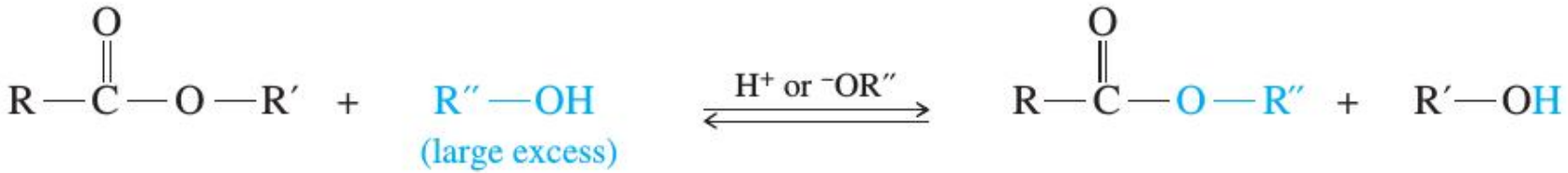
heptanoát



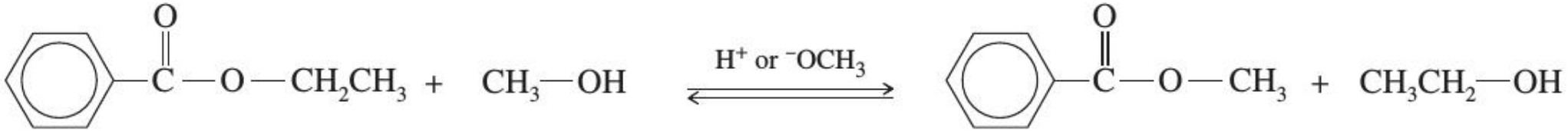
ciklohexánkarboxilát

Transzészterifikációs reakciók

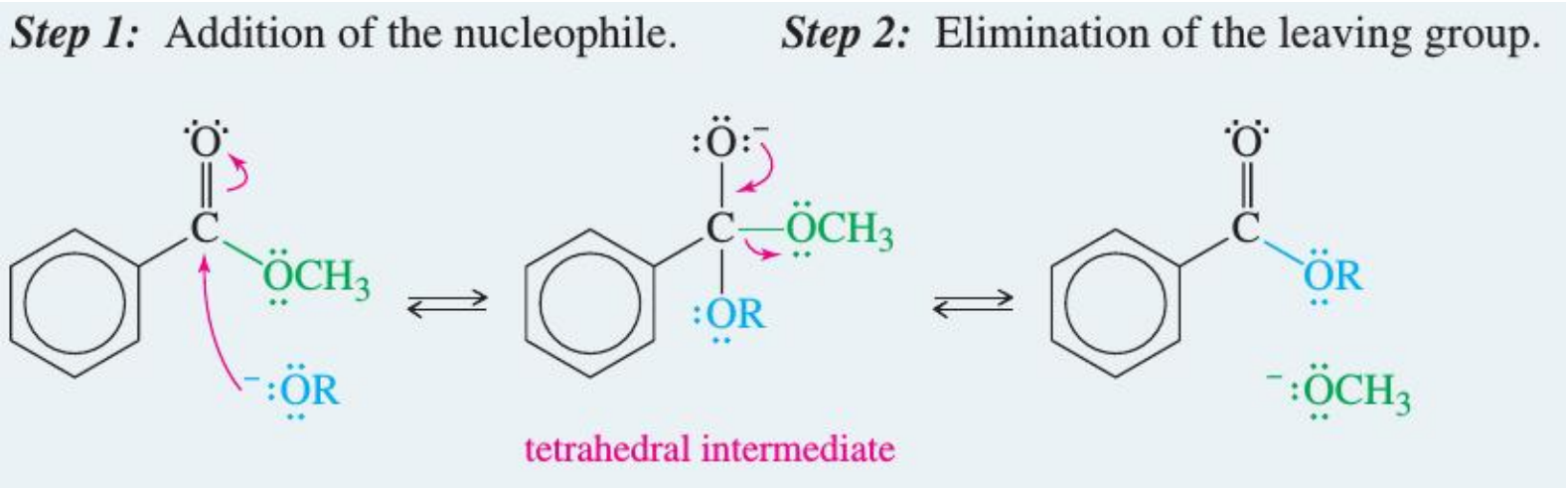
Egy észter másféle észterré történő konvertálása hidrolízis nélkül, közvetlenül alkohollal



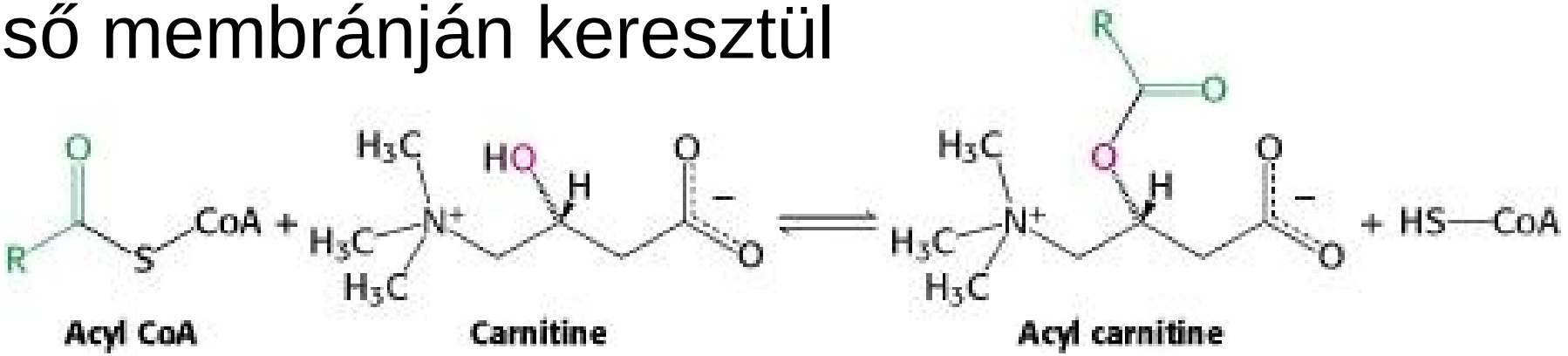
Example



Mechanizmus: nukleofil acil szubsztitúció

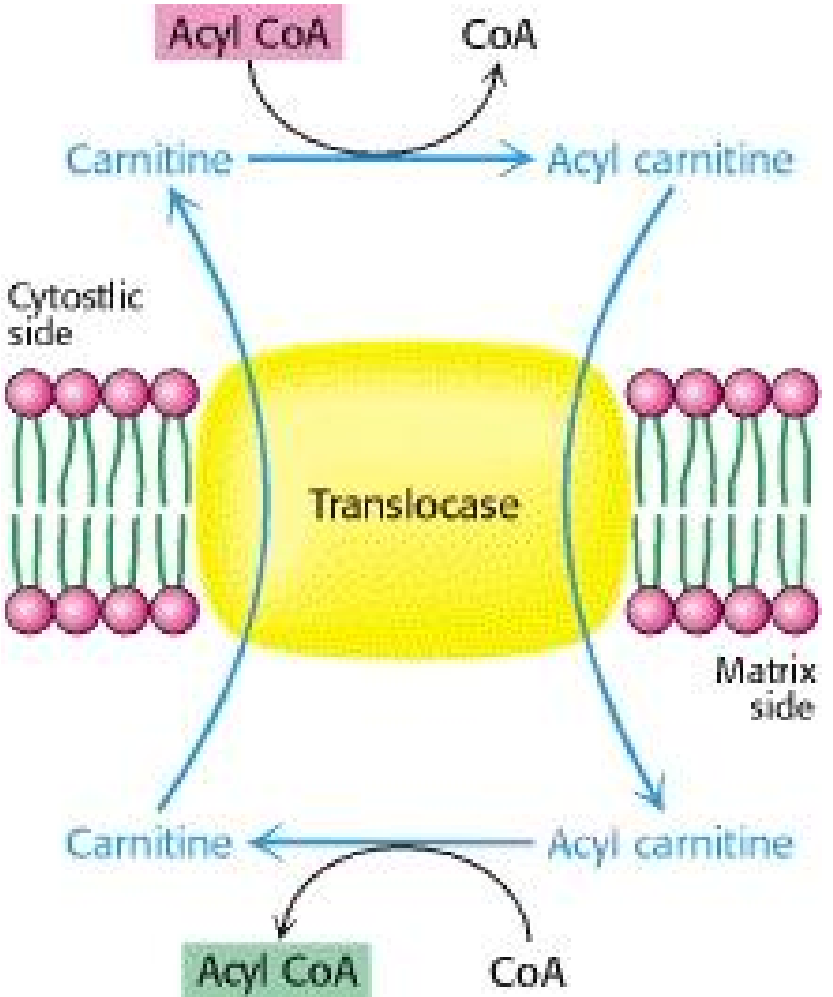


Kitekintés: zsírsavak transzportja a mitokondrium belső membránján keresztül



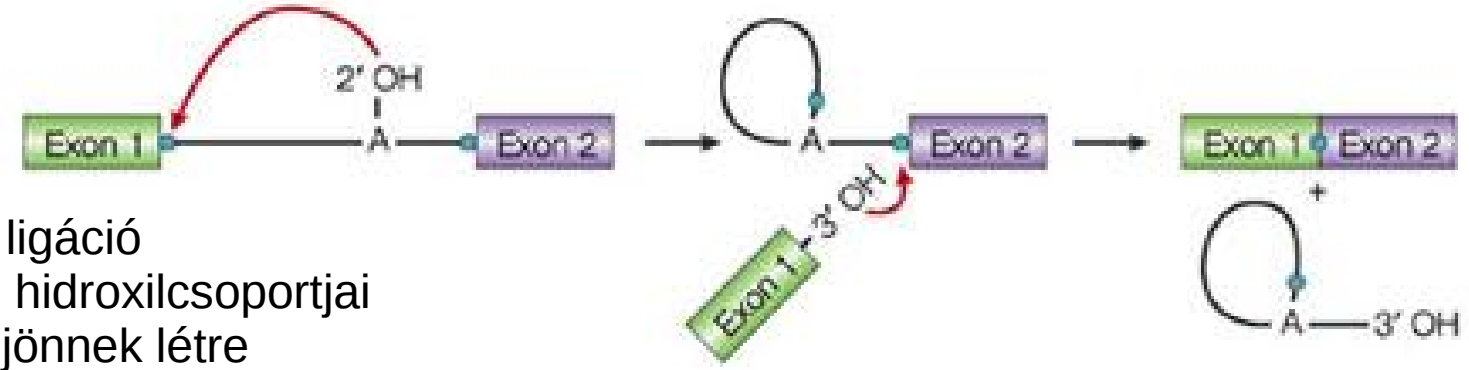
Transzészterifikációs reakciók észter és tioészter (lásd később) résztvevőkkel

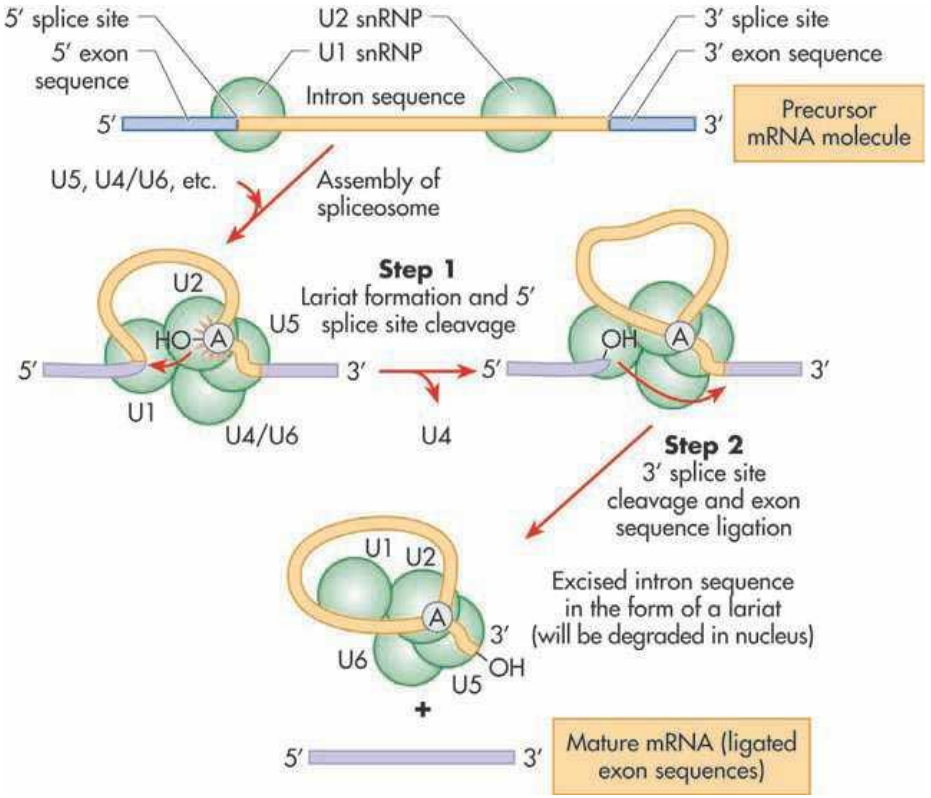
Az acil-koenzim A nem tud átjutni a membránon, csak a karnitin ill. az acil-karnitin.

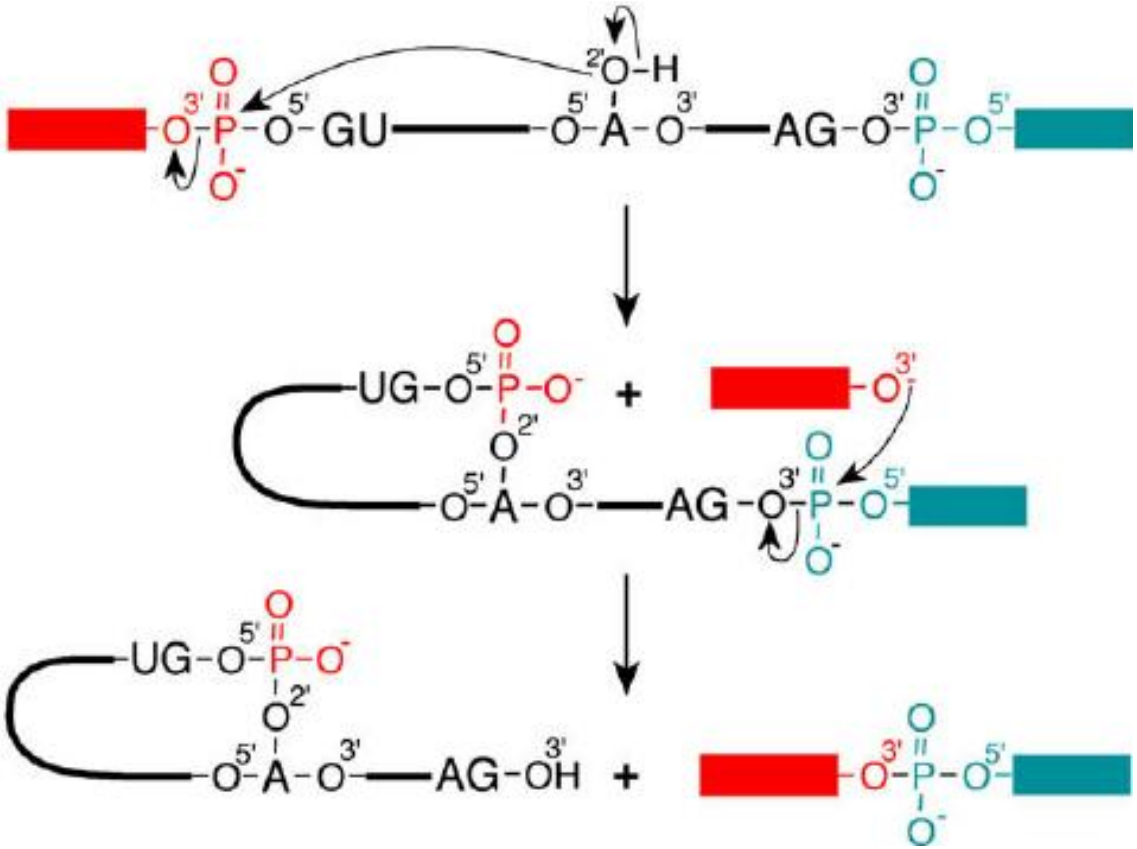


Kitekintés: a splicing

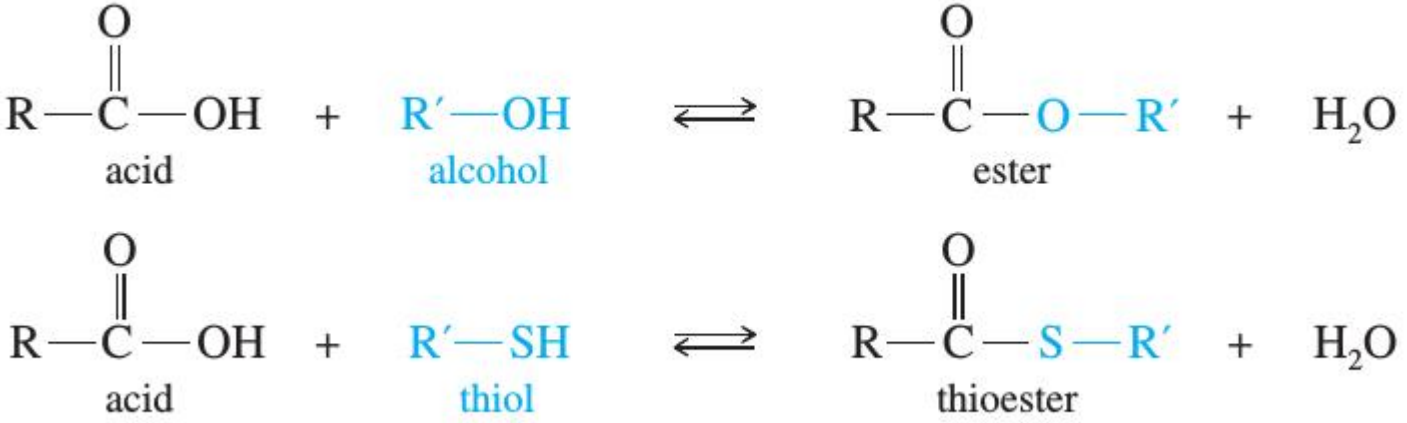
Intronok kivágása
mRNSből (lásd biokémia)
Két átésztereződési
reakció, nincs hidrolízis és ligáció
Az érintett észterek a ribóz hidroxilcsoportjai
és foszfátcsoportok között jönnek létre



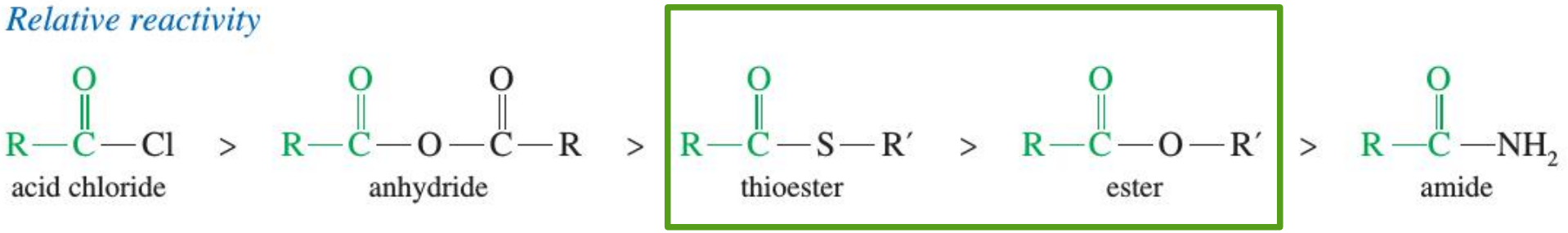




Tioészterek



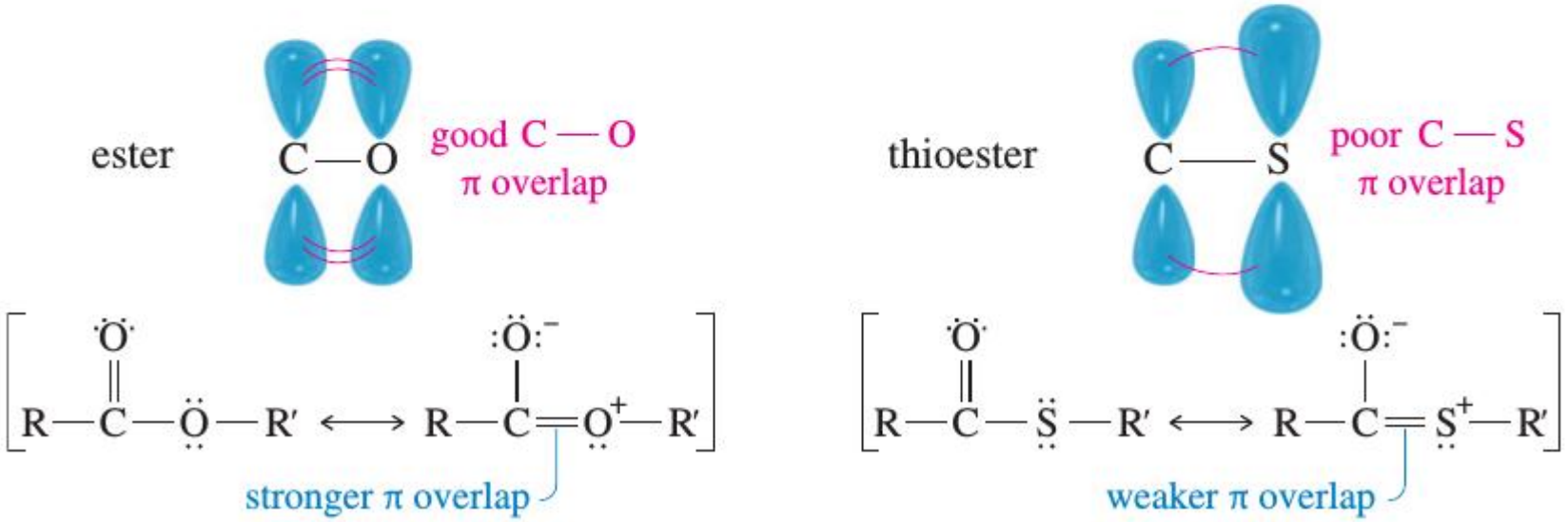
Az észterekkel analóg, de azoknál reaktívabb karbonsavszármazékok. Figyeljük meg, hogy a két szénatommal kötést kialakító oxigént helyettesítjük kénnel!



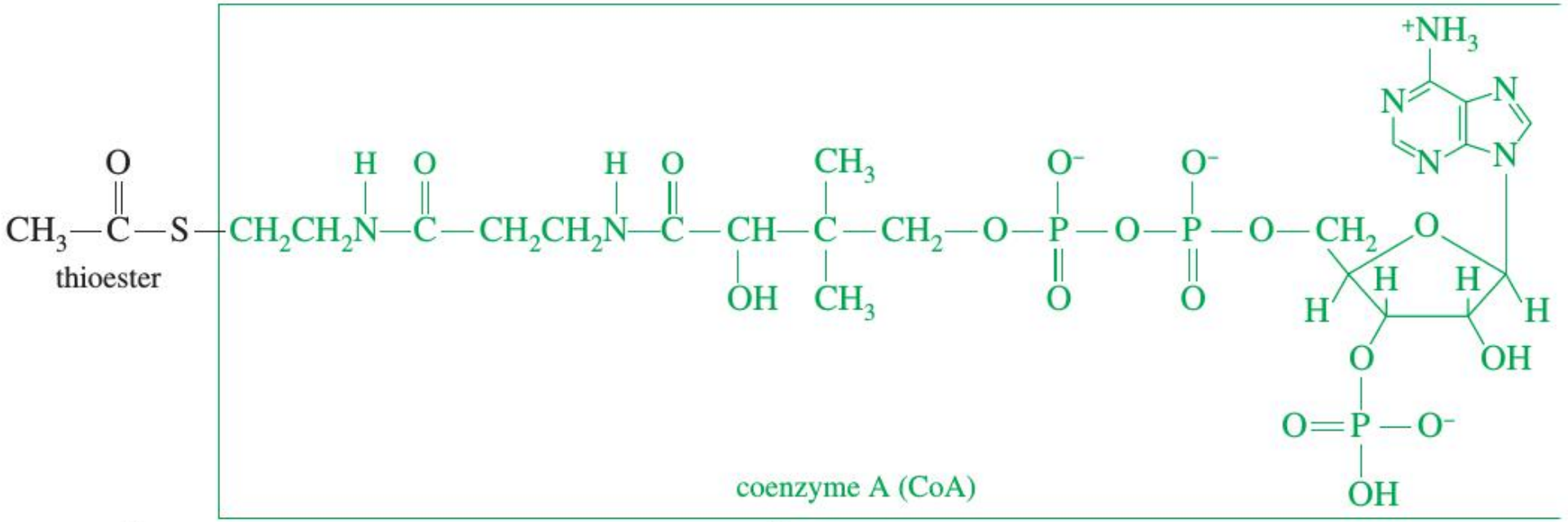
Kitekintés: tioészterek reaktivitása

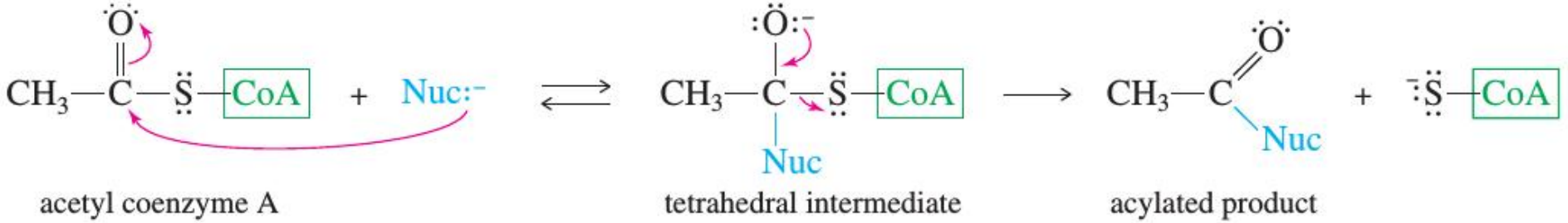
The enhanced reactivity of thioesters results from two major differences. First, the resonance stabilization of a thioester is less than that of an ester. In the thioester, the second resonance form involves overlap between a $2p$ orbital on carbon and a $3p$ orbital on sulfur (Figure 21-12). These orbitals are different sizes and are located at different distances from the nuclei. The overlap is weak and relatively ineffective, leaving the C—S bond of a thioester weaker than the C—O bond of an ester.

The second difference is in the leaving groups: An alkyl sulfide anion ($^{-}:\ddot{\underset{\cdot\cdot}{S}}—R$) is a better leaving group than an alkoxide anion ($^{-}:\ddot{\underset{\cdot\cdot}{O}}—R$) because the sulfide is less basic than an alkoxide, and the larger sulfur atom carries the negative charge spread



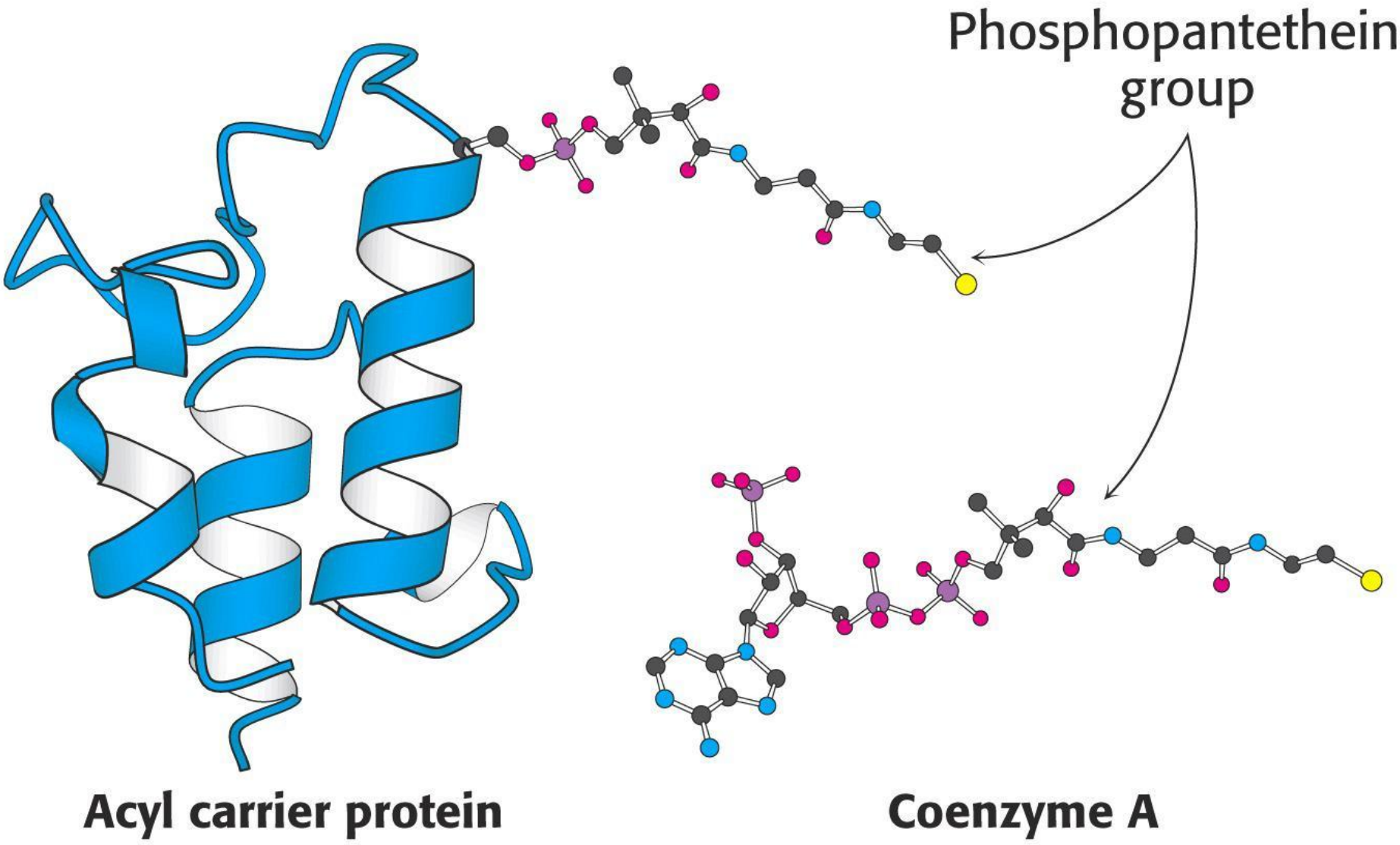
Kitekintés: tioészterek a biokémiában





Citromsav-cikus, zsírsavlebontás

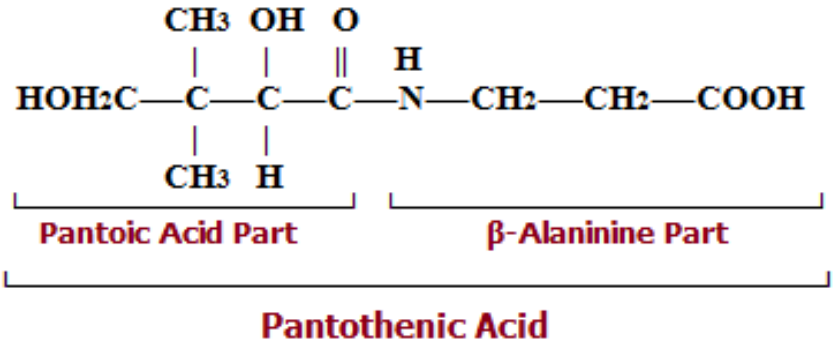
Kitekintés: tioészterek a biokémiában

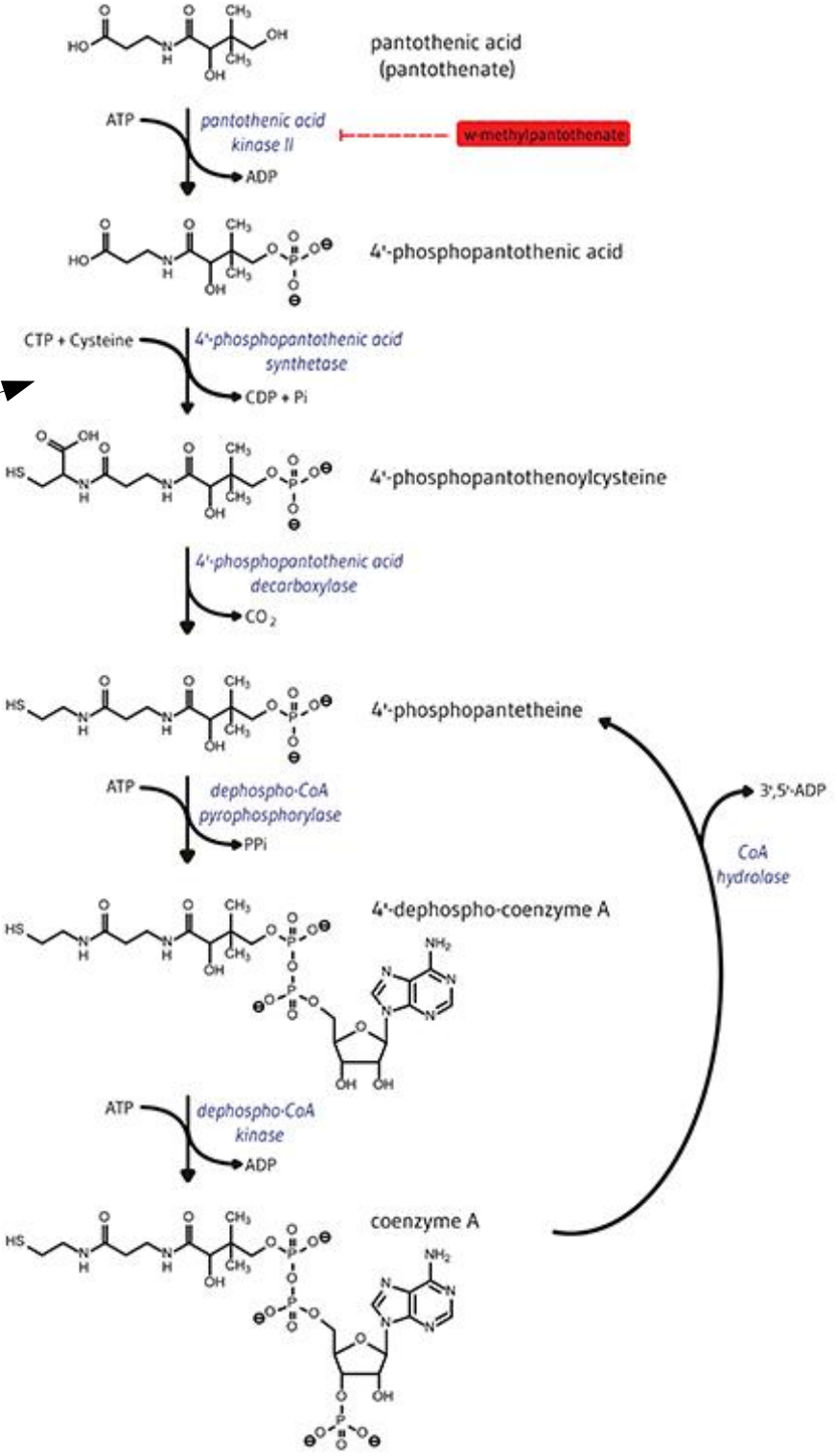


Zsírsavszintézis: acetil-koenzim A → acetil-ACP: tioészterek közötti átésztereződés

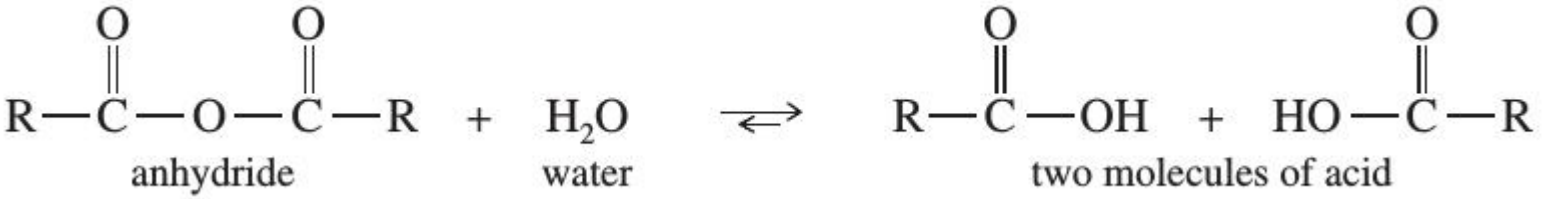
Kitekintés: tioészterek a biokémiában

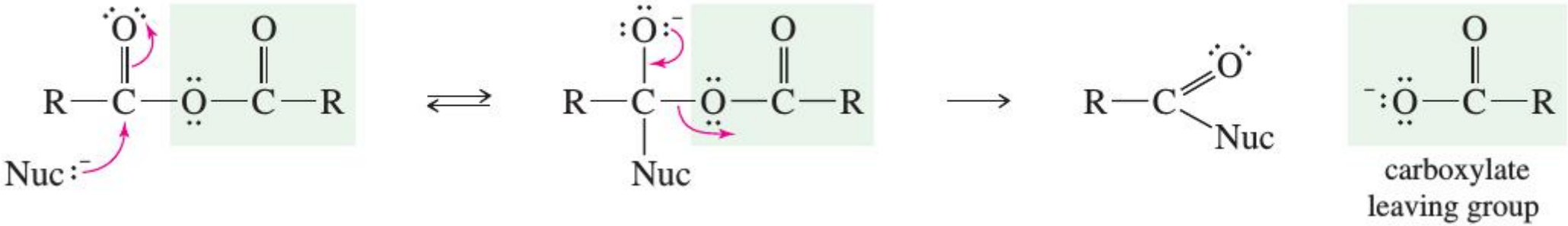
Az SH csoport ciszteinből, a hordozó “kar” többi része a B5-vitaminnak megfelelő pantoténsavból származik





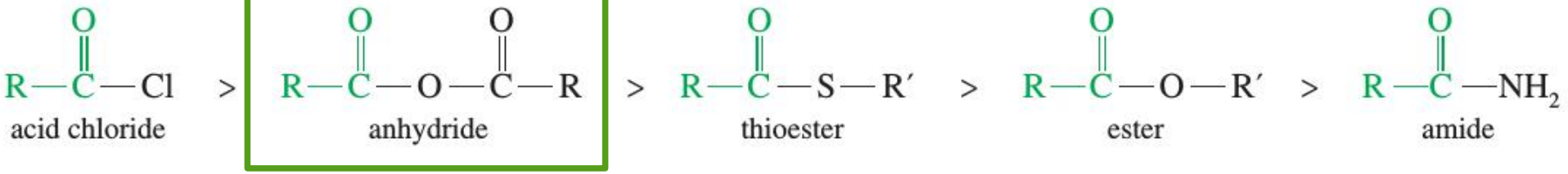
Savanhidridek





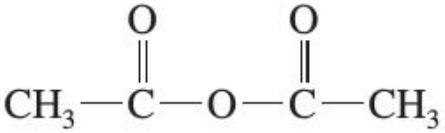
A tioészthereknél is reaktívabb karbonsavszármazékok, két karboxilcsoportból vízelvonással származtathatóak.

Relative reactivity

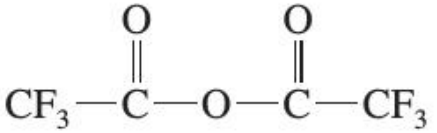


Savanhidridek

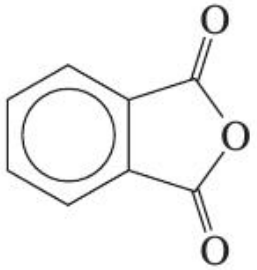
A két karboxilcsoport származhat két molekulából, ebben az esetben az anhidrid lehet szimmetrikus vagy aszimmetrikus, illetve származhat egy molekulából is, ebben az esetben intramolekuláris / gyűrűs anhidridről beszélhetünk.



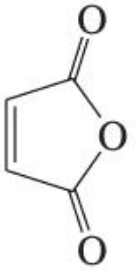
(abbreviated Ac_2O)
ethanoic anhydride
acetic anhydride



(abbreviated TFAA)
trifluoroethanoic anhydride
trifluoroacetic anhydride

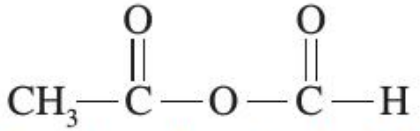


benzene-1,2-dicarboxylic anhydride
phthalic anhydride

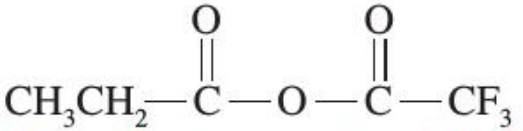


but-2-enedioic anhydride
maleic anhydride

Anhydrides composed of two different acids are called **mixed anhydrides** and are named by using the names of the individual acids.

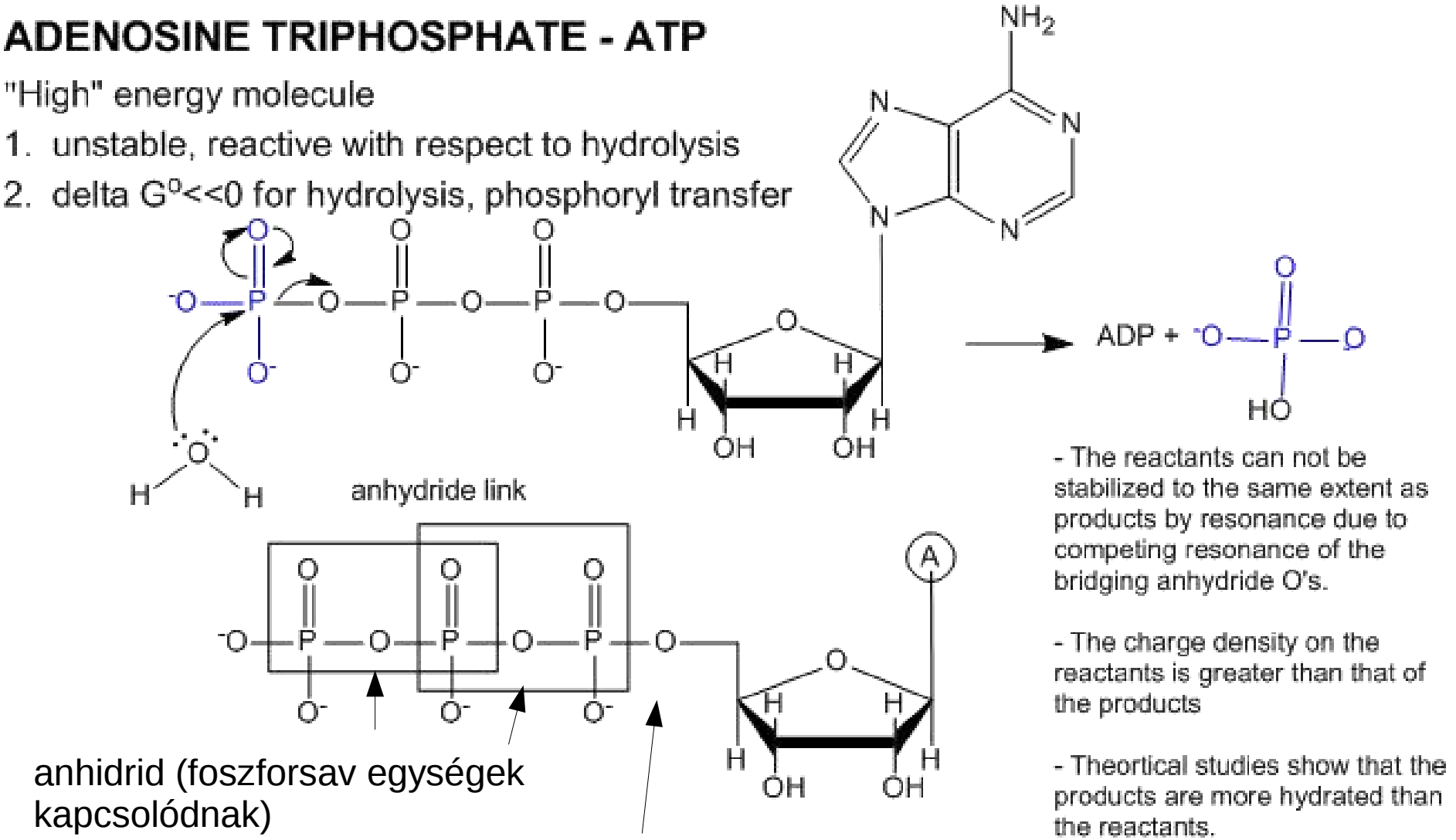


IUPAC name: ethanoic methanoic anhydride
common name: acetic formic anhydride



trifluoroethanoic propanoic anhydride
trifluoroacetic propionic anhydride

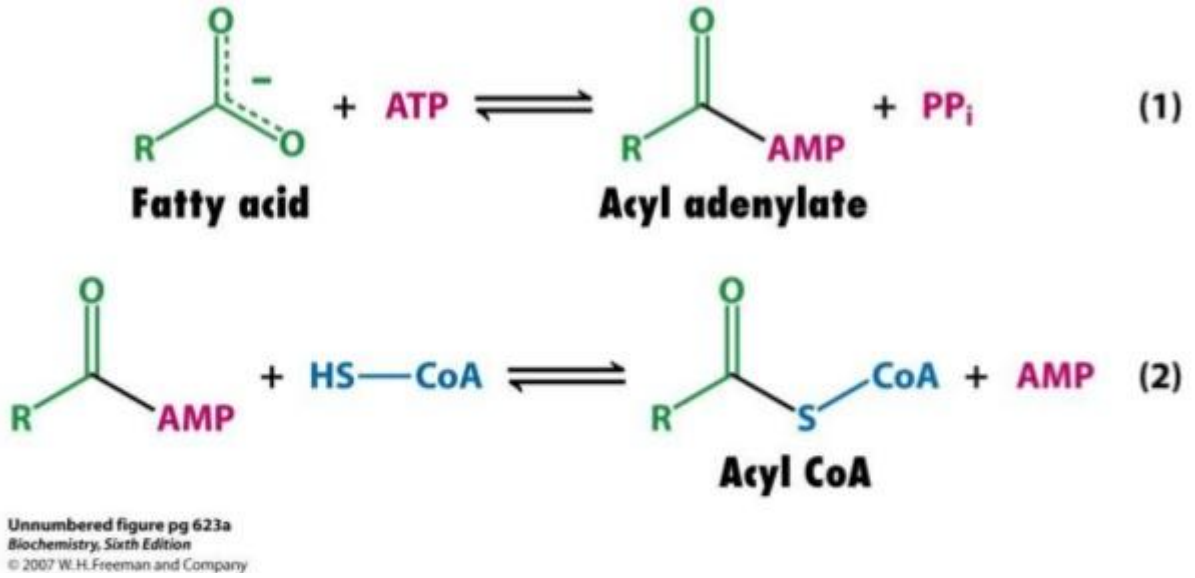
Szervetlen és vegyes savanhidridek – az ATP példája



anhidrid (foszforsav egységek kapcsolódnak)

észter (foszforsav és hidroxilcsoport kapcsolódik)

Kitekintés: karboxilcsoport “aktiválásának” általános biokémiai mechanizmusa

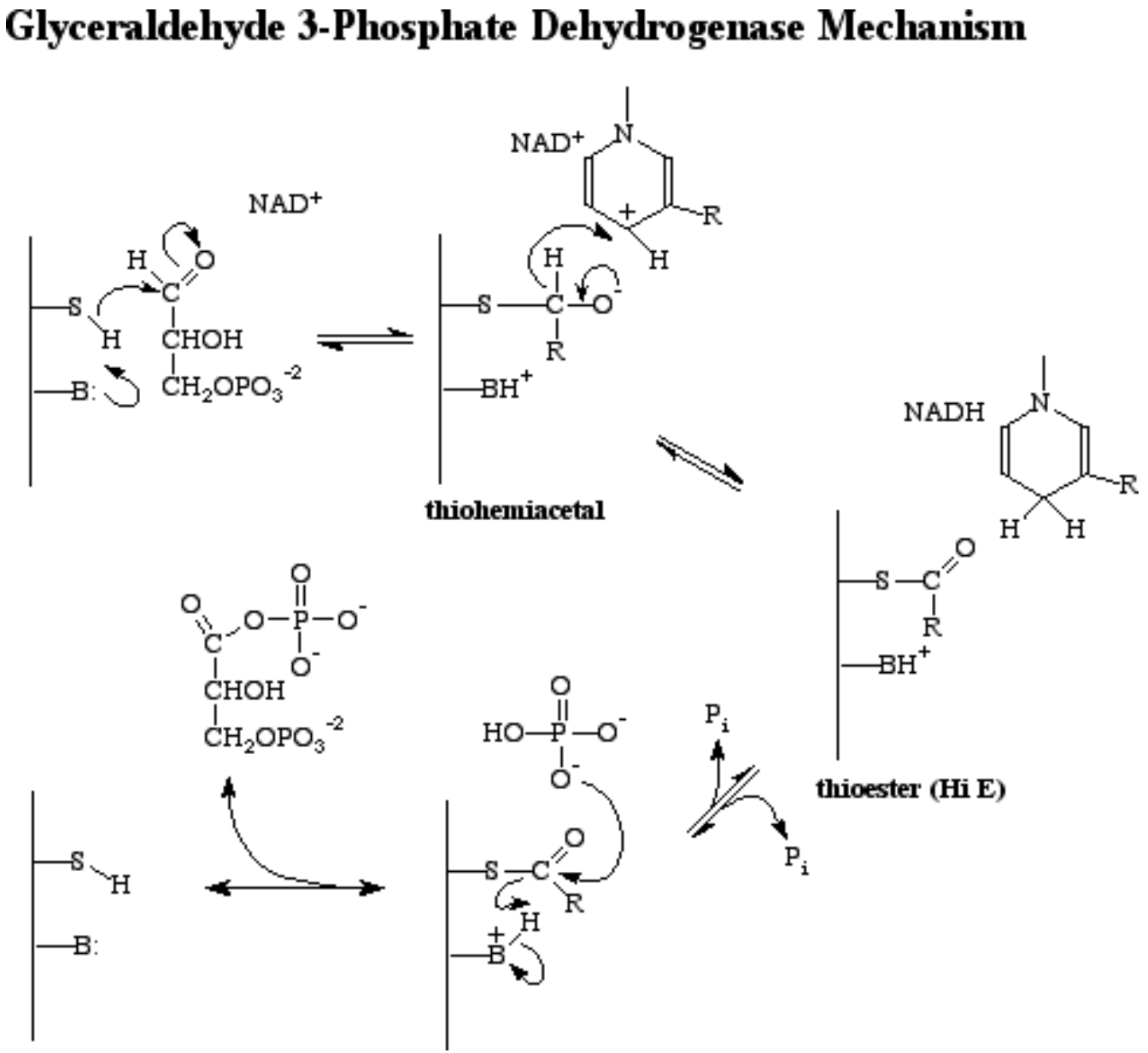


Vegyes anhidrid (képződéséhez ~2 ATP ekvivalens használódik el)

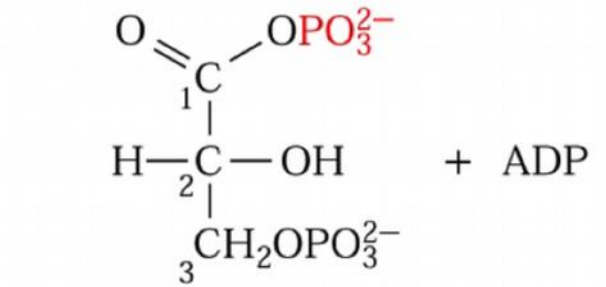
Tioészter (egyéb esetekben lehet észter)

Karbonsav	Acilcsoport akceptor	Folyamat
aminosav	tRNS	transzláció
zsírsav	koenzim A	zsírsavlebontás
acetát	koenzim A	glioxalát ciklus
ubiquitin (egy fehérje)	E1 (egy fehérje)	ubiquitináció

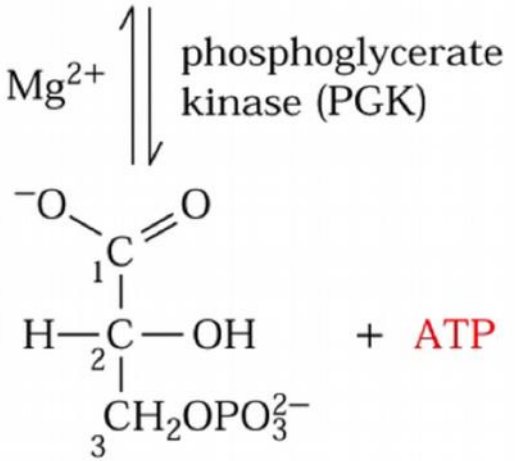
Kitekintés: a glikolízis két egymás utáni lépése



Aldehidcsoport oxidációja kabonsavszármazékká (vegyes anhidrid!) - két nukleofil acil szubsztitúciós lépés!



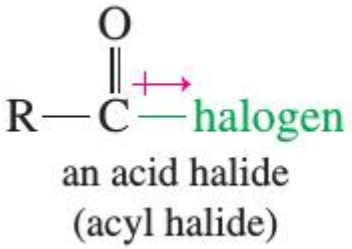
1,3-Bisphosphoglycerate (1,3-BPG)



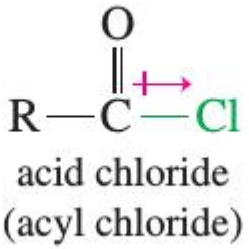
3-Phosphoglycerate (3PG)

A következő lépésben a foszfátcsoport ADP-re kerül át: karbonsav és ATP képződik – tiszta nyereség!

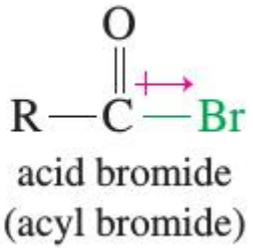
Savhalogenidek



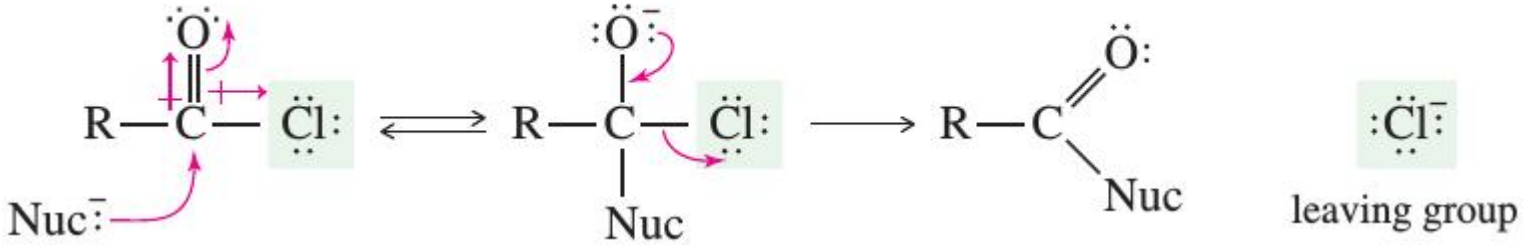
an acid halide
(acyl halide)



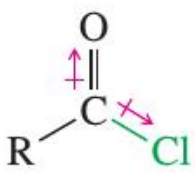
acid chloride
(acyl chloride)



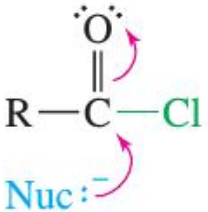
acid bromide
(acyl bromide)



A halogén elektronszívó hatása növeli a karbonil szén elektronszegény jellegét, ezáltal jobb célponttá téve nukleofil ágensek támadásához.

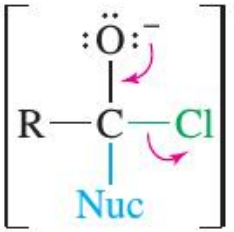


an acid chloride (acyl chloride)



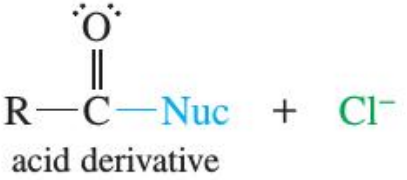
acid chloride

addition



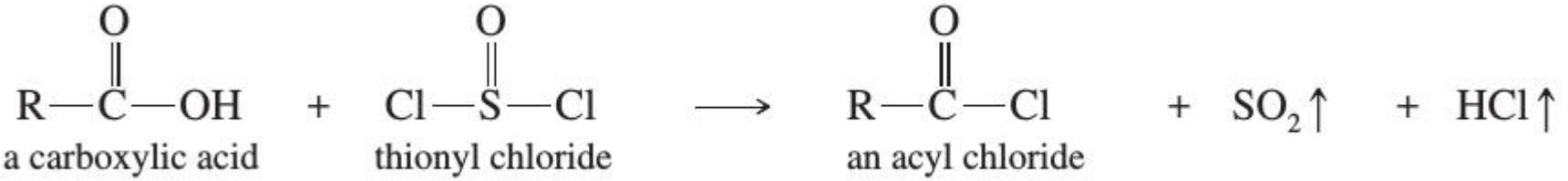
tetrahedral intermediate

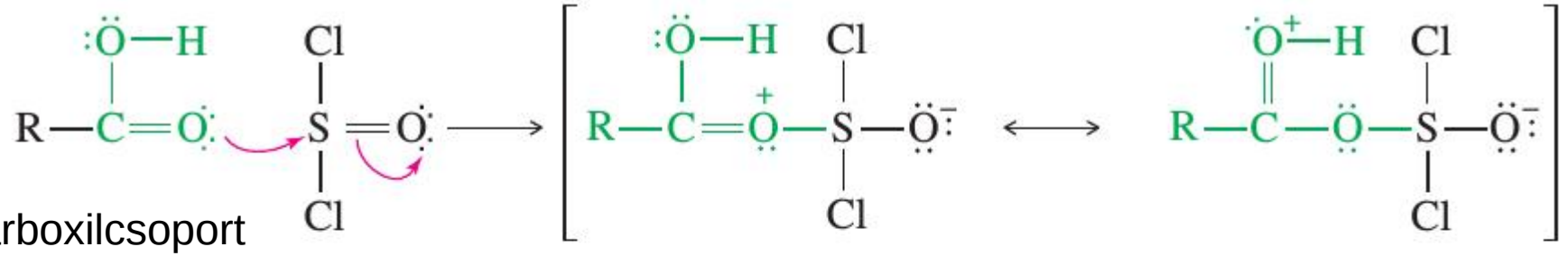
elimination



acid derivative

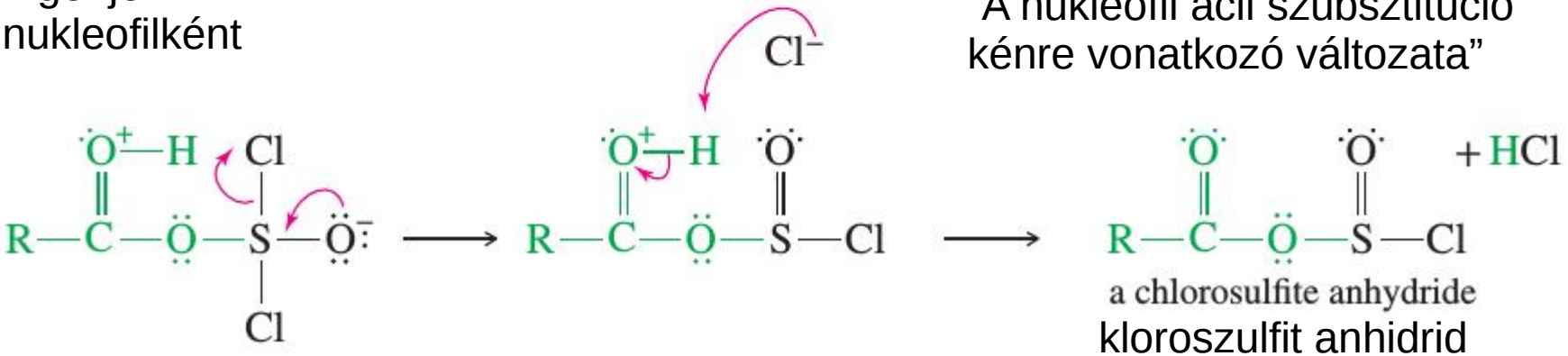
Kitekintés: savhalogenidek előállítása

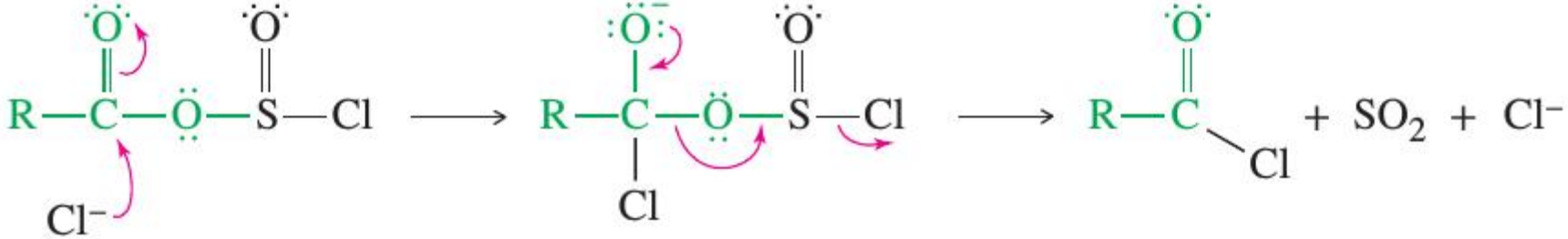




A karboxilcsoport egyik oxigénje támad nukleofilként

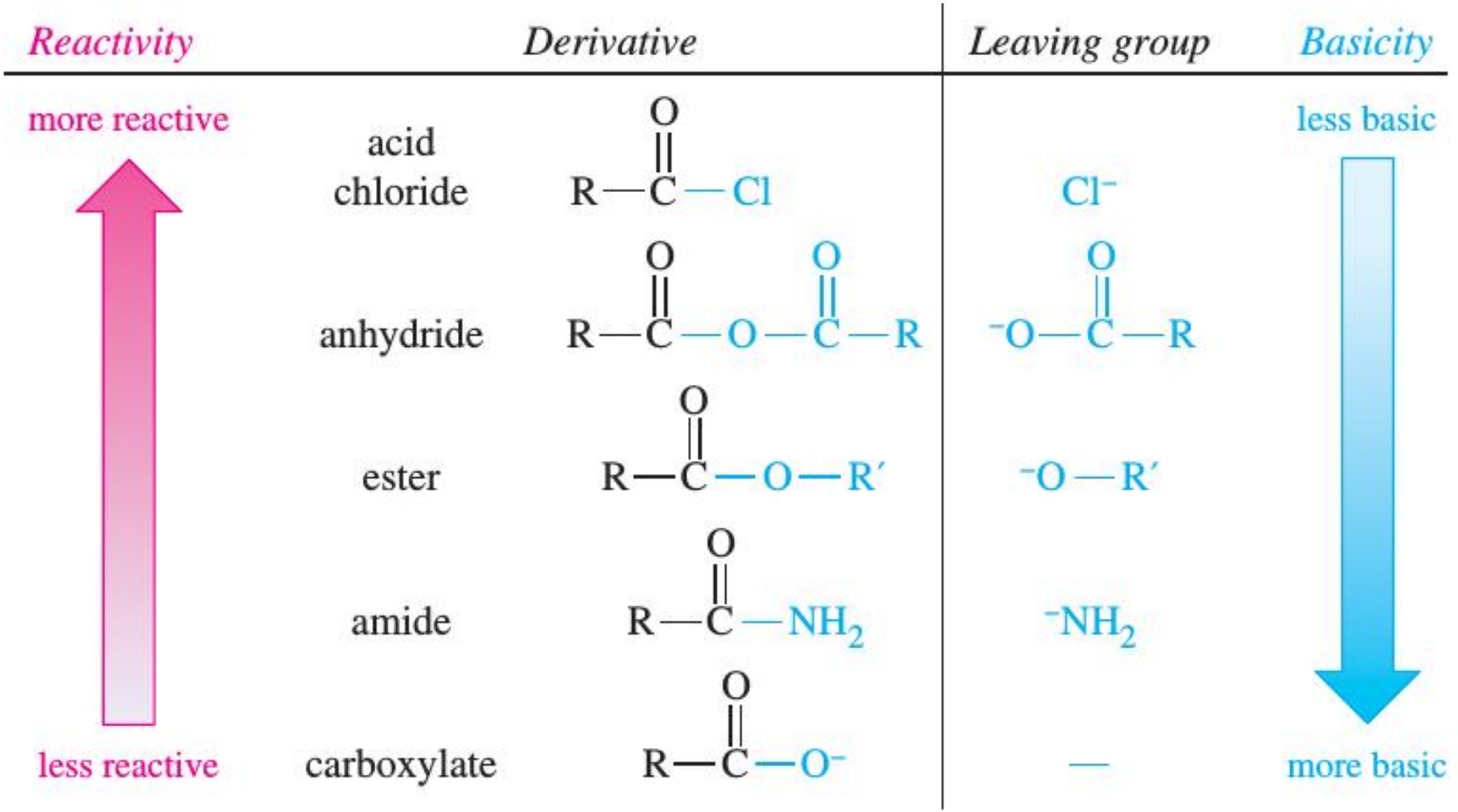
“A nukleofil acil szubsztitúció kénre vonatkozó változata”



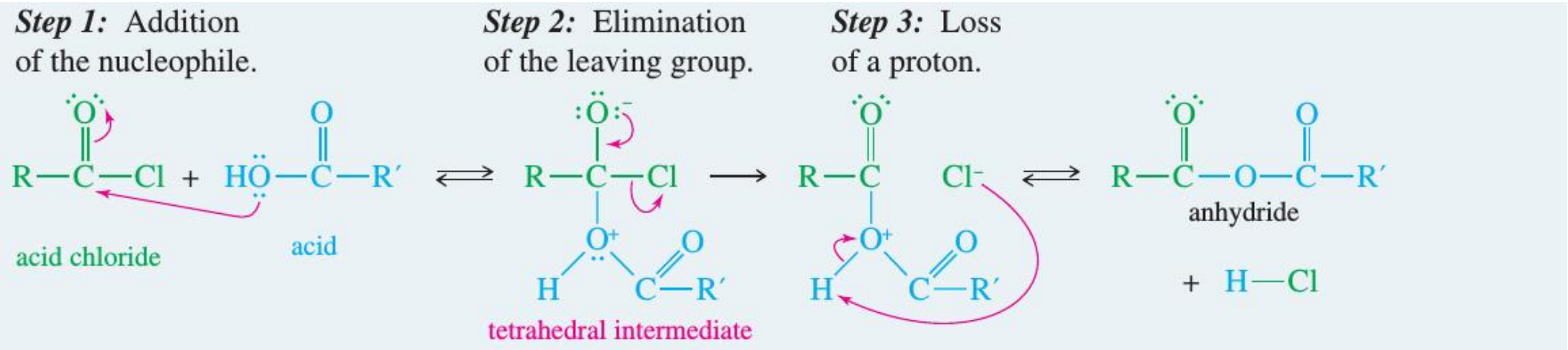


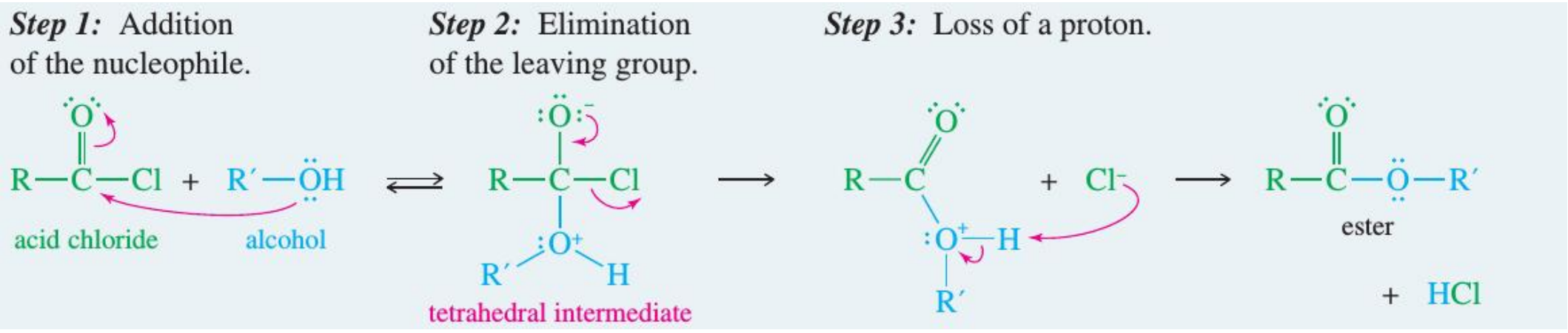
Majd a köztitermék egy Cl^- nukleofil acil szubsztitúja révén alakul savkloriddá

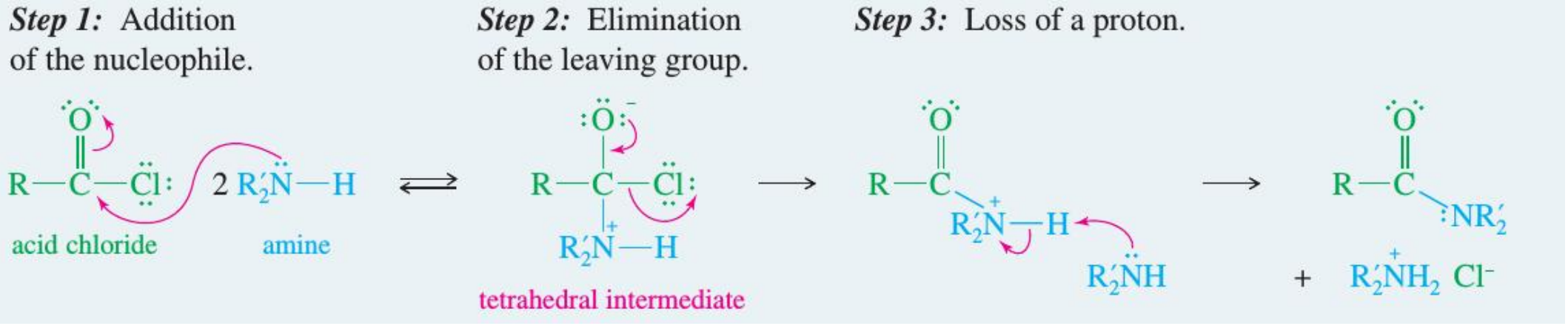
Fontosabb karbonsavszármazékok reaktivitása



Nukleofil acil szubsztitúció savhalogenidekkel







Mit kell tudni?

- Karboxilcsoport, karbonsavak értékűsége
- A karbonsavak és halogénezett karbonsavak savassága
- Karbonsavak sói
- A dekarboxileződés (mechanizmus nélkül)
- A nukleofil acil szubsztitúció elve, legalább egy mechanizmus lépései
- Észterek: szerkezet, képződés (elv), hidrolízis (elv), transzészterifikáció (elv), laktonok
- Anhidridek levezetése
- Tioészterek, savhalogenidek és reaktivitásuk a karboxilcsoporthoz képest