

XV. Heterociklusos szénvegyületek:

Stabilitás:

A benzol esetében jóslott ($3 \cdot -28.6$) ΔH -hoz képest a mért hidrogénezési „hő” jelentős stabilitásra utal (-36). A piridin esetében a rezonancia energia kisebb (-27) és az tovább csökken a pirrolnál (-22).

legfontosabb faktor:

1) **elektronegativitás**

C(2.5), S(2.5),

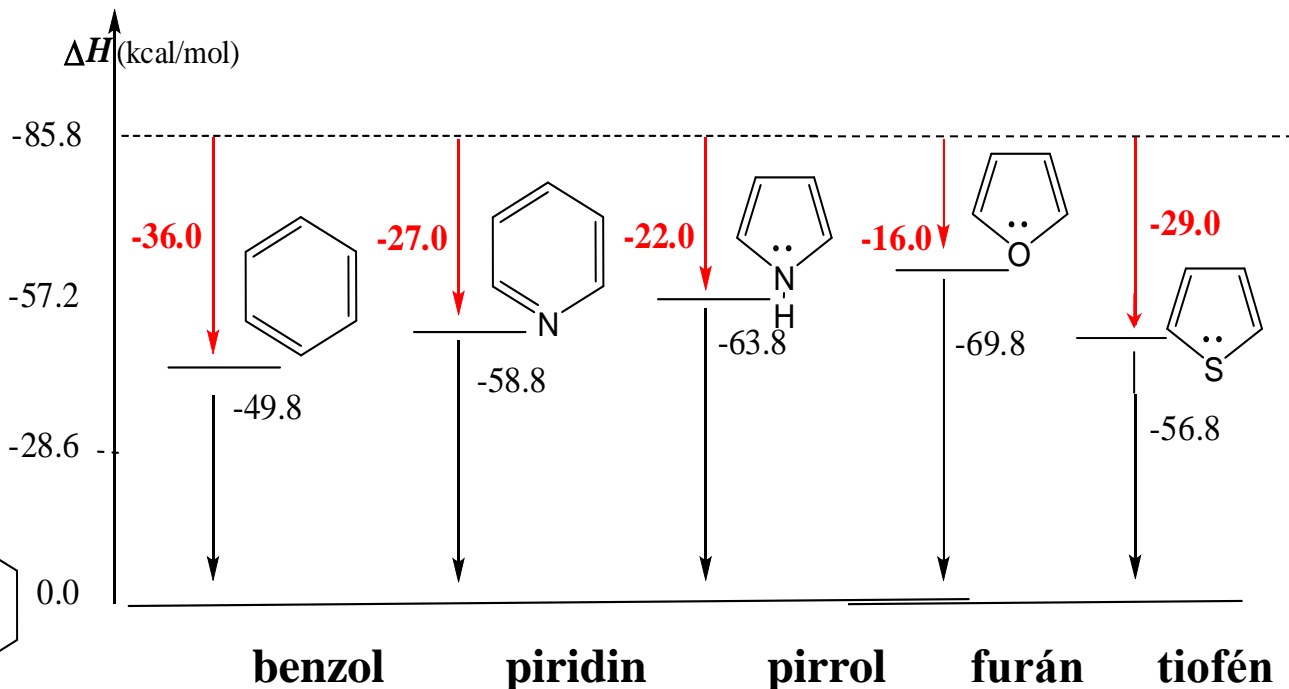
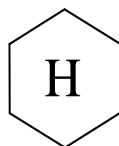
N(3.0), O(3.5)

valamint a

2) **heteroatom mérete:**

S(1.83Å), C(1.70 Å), N

(1.55Å), O(1.52Å))

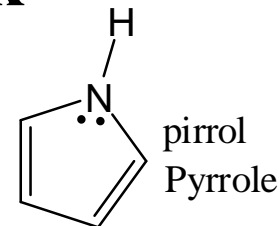
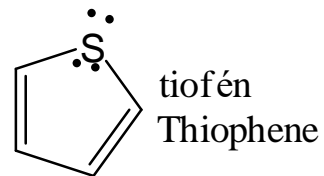
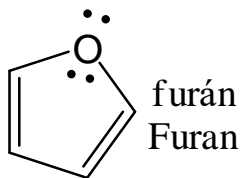


tipikus reakciók:

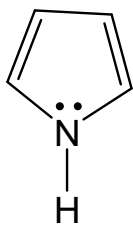
A benzolhoz hasonlóan a piridin, pirrol, furán, tiofén is inkább S_E és *nem* addíciós reakcióban vesz részt. Mind az öt vegyület aromás.

XV. Egy heteroatomos öttagú gyűrűk

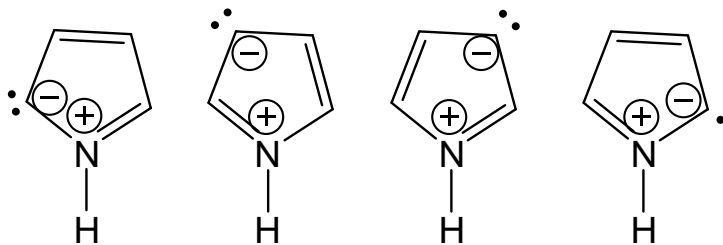
aromás molekulák:



apoláris határszerkezetek



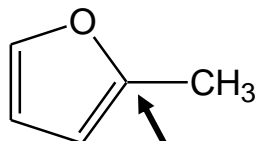
poláris határszerkezetek



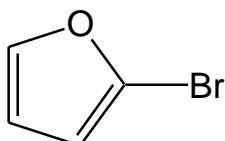
benzolhoz képest :
magnövekedett reaktivitás!

1. A furánvázis vegyületek

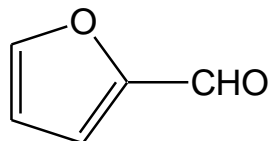
A. Furán szubsztituált származékai



2-metilfurán
2-Methylfuran

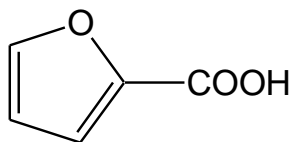


2-brómfurán
2-Bromofuran

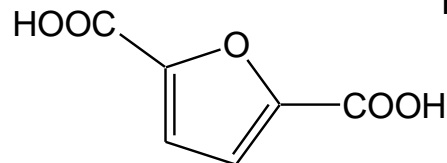


furán-2-karbaldehid
(furfurol)
Furan-2-carbaldehyde

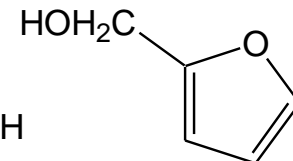
1-es C nincs!



furán-2-karbonsav
(pironyálkasav)
Furan-2-carboxylic acid

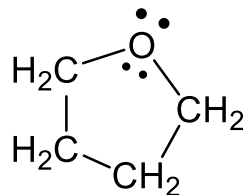


furán-2,5-dikarbonsav
(dehidronyálsav)
Furan-2,5-dicarboxylic acid



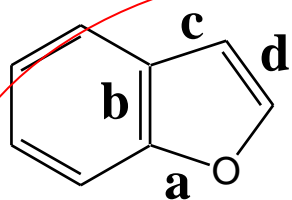
2-(hidroximetil)furán
(furfurilalkohol)
(2-furyl)methanol

B. Telített furánszarmazékok



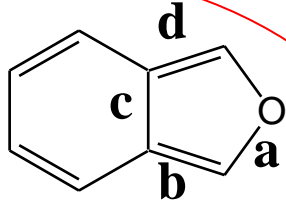
tetrahidrofurán
Tetrahydro-furan

C. A furán benzológjai



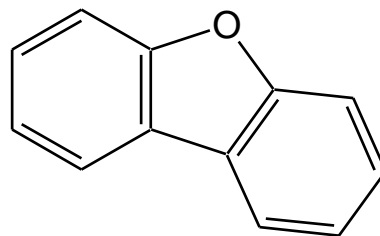
benzofurán
benzo[b]furán
kumaron

Benzofuran



izobenzofurán
benzo[c]furán

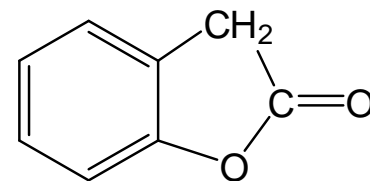
Isobenzofuran



dibenzofurán

Dibenzofuran

Példa:

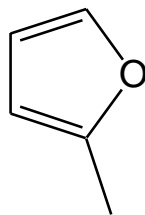


2-kumaron
kumarán-2-on

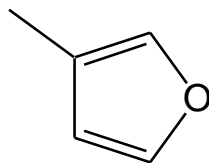
3*H*-Benzofuran-2-one

Szerkezeti izomerek

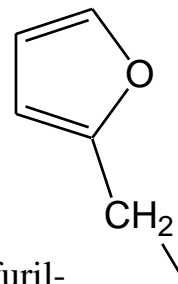
D. Csoportnevek



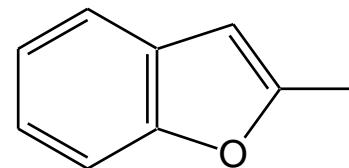
2-furil-



3-furil-



furfuril-



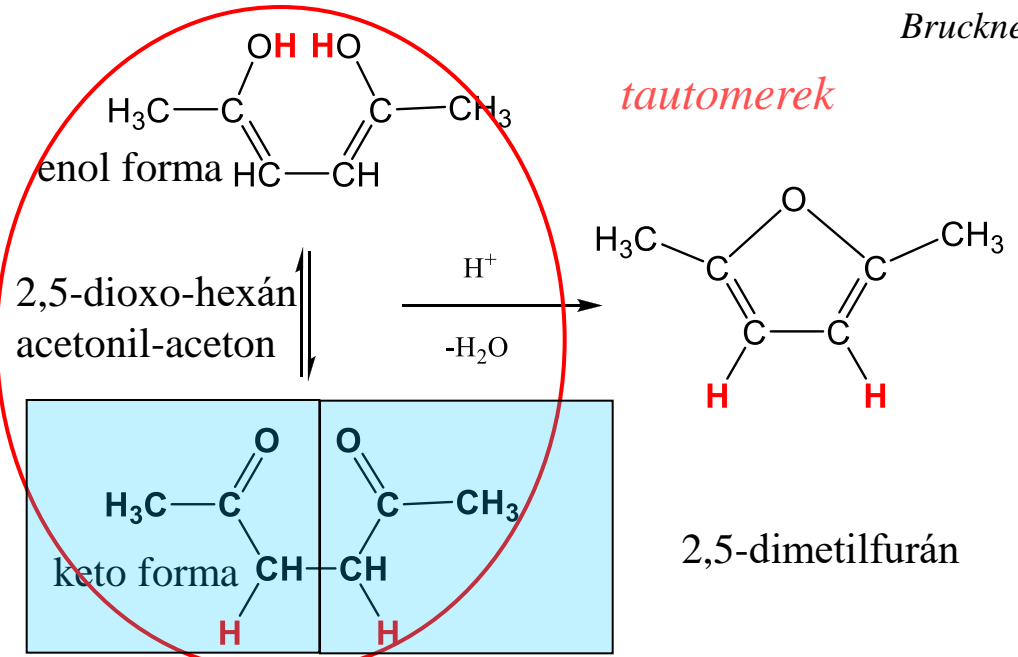
2-benzofuranil-

példa: két példa furán származék (egy heteroatomos öttagú heterociklusos vegyület) előállítására

A furán előállítása:

kiindulási anyag:

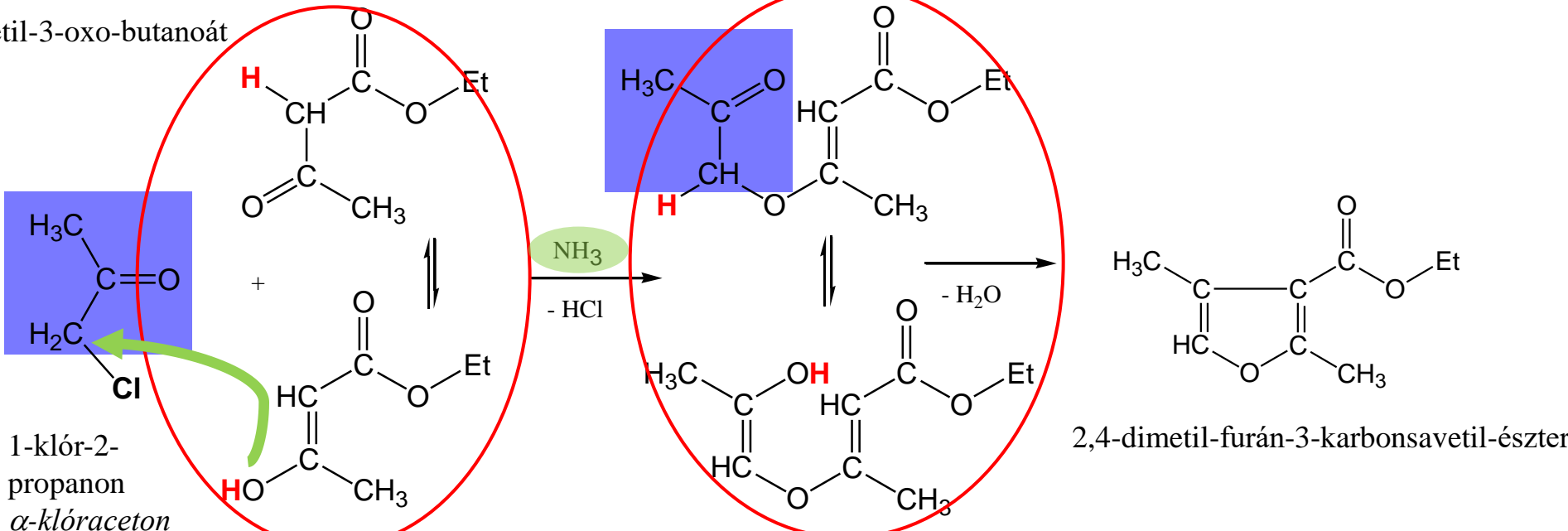
2,5-diketon vagy
1,4-dialdehid



tautomerek

egy másik szintézis α-halogénezett ketonokból:

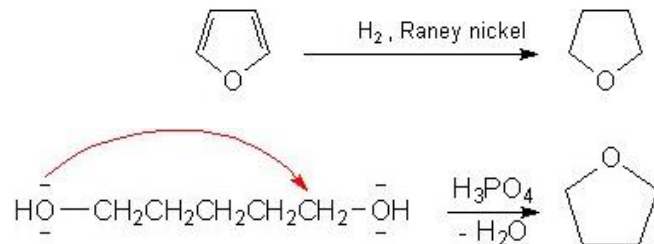
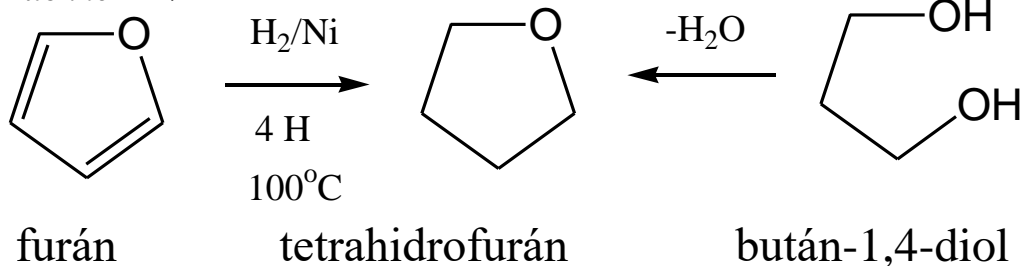
etil-3-oxo-butanoát



1-klór-2-propanon
α-klóraceton

két eljárás a tetrahydrofuran előállítására:

Bruckner III/41



Bruckner III/74

Példák furánvázis természetes vegyületekre:

1) **uzninsav** (op: 204°)

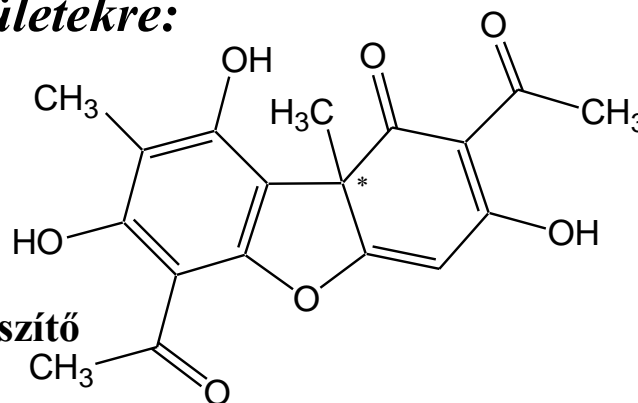
(dibenzofurán származék):

sárga színű, keserű **növényi pigment**

zuzmókban fordul elő,

antibiotikus hatású, UV abszorbens

krém, deo, sampon, fogkrém + étrend-kiegészítő



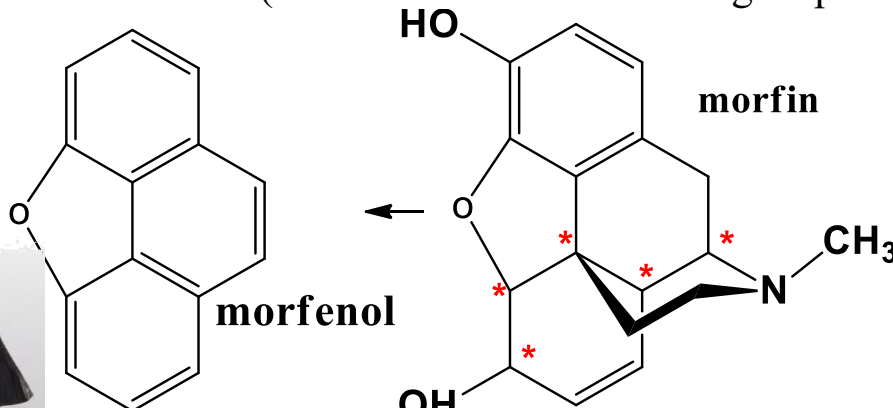
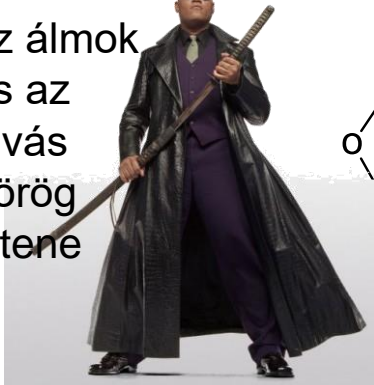
Bruckner III/75, 938

2) **morfenol** (op: 145°) (Vongerichten 1901)

morfin lebontási terméke (a morfin szerkezetének megállapításában fontos szerepe volt)

Morpheus

az álmok
és az
alvás
görög
istene



lehetséges sztereo-izomerek száma?

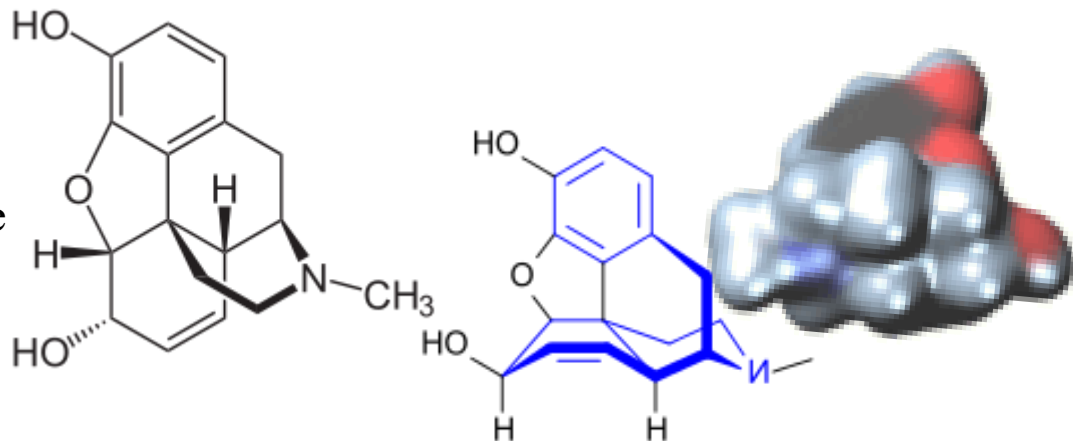
morfin: az ópium főalkaloidja
(Sertürner 1805)

Az ópiumból izolált rokon
alkaloidok: **kodein** [metoxi-
morfin], **tebain** [dimetoxi-morfin]

fiziológiás hatás:

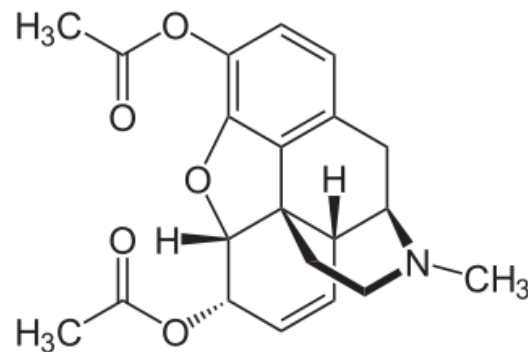
fájdalomcsillapító, euforikus
hatású, altató, stb..

1827 Merck: morfin – ópium és
- alkoholfüggőség
kezelésére



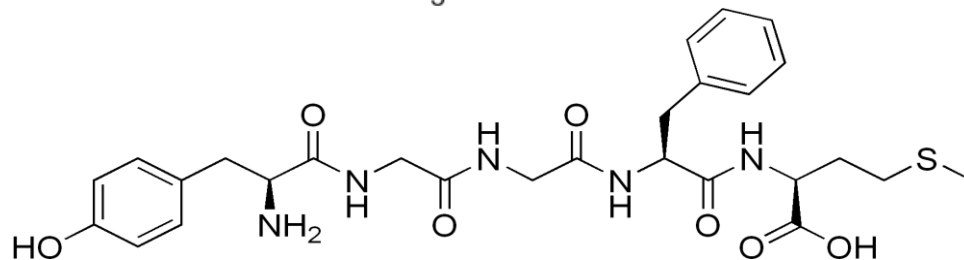
1874 Bayer: diacetil-morfin (heroin)

- morfinfüggőség kezelésére
- köhögés-gátló
- 1,5-2x hatékonyabb
- gyorsabban jut át a vér-agy gáton



2003 endogén morfin:

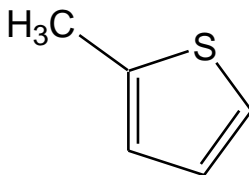
- μ_3 -opioid receptor



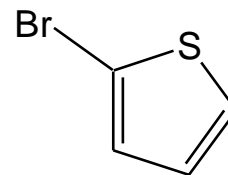
met-enkefalin (egy endorfin-molekula)

2. Tiofénvázás vegyületek

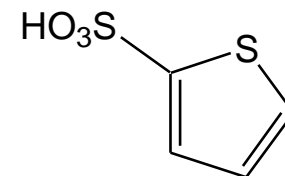
A. A tiofén szubsztituált származékai



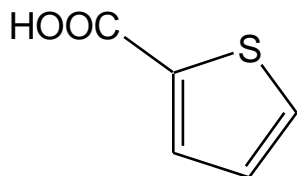
2-metiltiofén
2-Methylthiophene



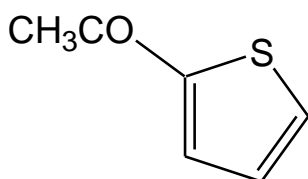
2-brómtiofén
2-Bromothiophene



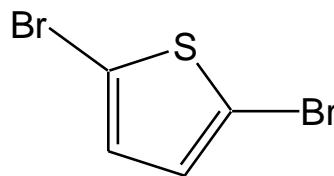
tiofén-2-szulfonsav
Thiophene-2-sulfonic acid



tiofén-2-karbonsav
Thiophene-2-carboxylic acid

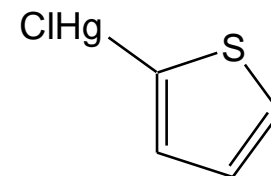


2-acetiltiofén
2-Acetylthiophene



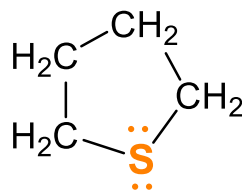
2,5-dibrómtiofén
2,5-Dibromothiophene

Példa: fémorganikus vegyület



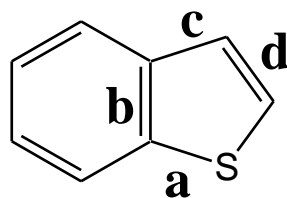
2-(klórmerkuri)tiofén

B. Telített tiofén származékai

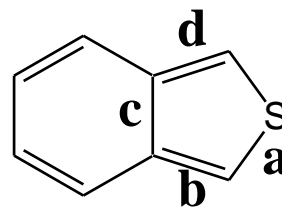


tetrahidrotiofén
Tetrahydrothiophene

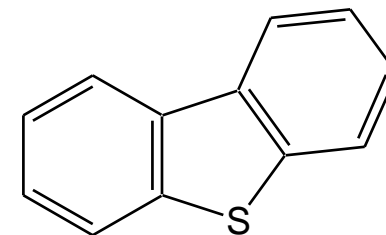
C. A tiofén benzológjai



benzo[b]tiofén
Benzo[b]thiophene

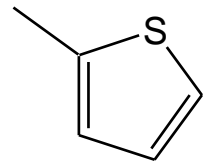


benzo[c]tiofén
Benzo[c]thiophene

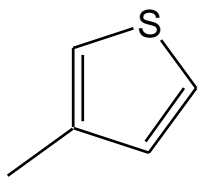


dibenzo-tiofén
Dibenzothiophene

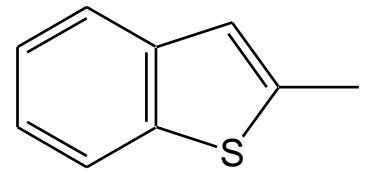
D. Csoportnevek



2-tienil-

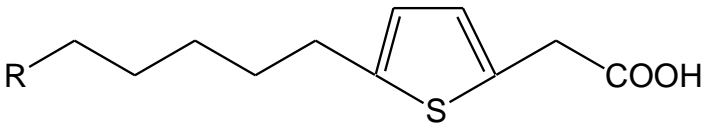


3-tienil-

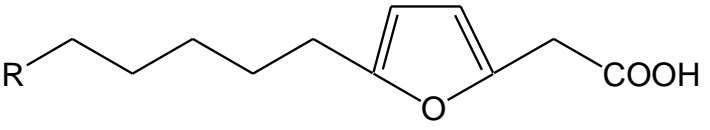


2-benzo[b]tienil-

Példa: tiofénvázas természetes vegyületekre

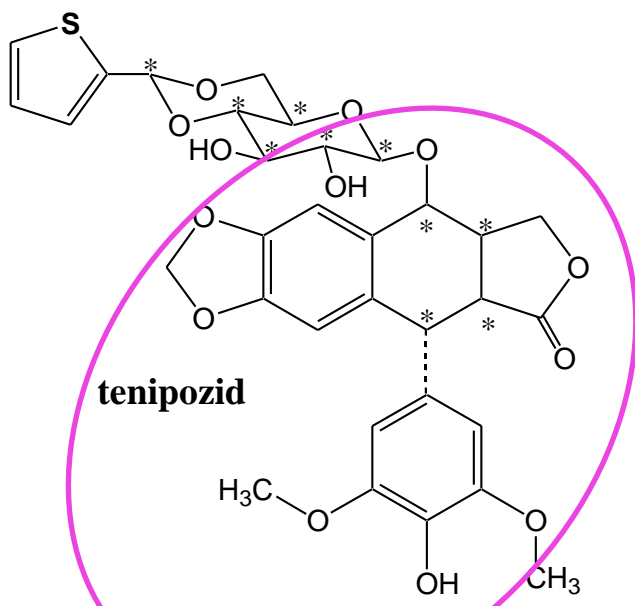


tiofén-származék

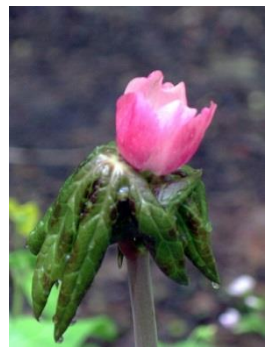


furán-származék

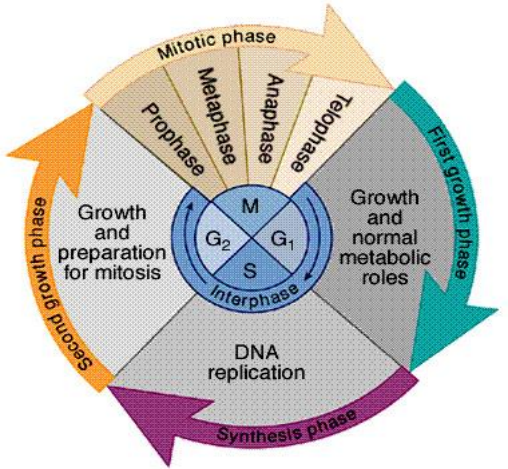
[NÉT1 207]



tenipozid



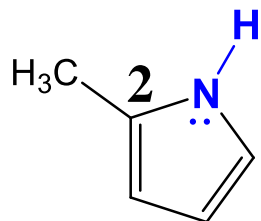
Podophyllum



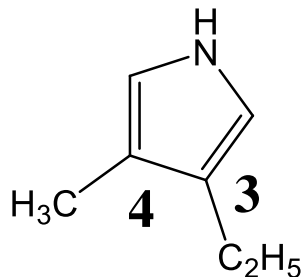
memo: általánosan használt sejtciklus gátlószer
terápiás profil: leukémiás betegeknél alkalmazzák, mivel gátolja a csontvelőben a vörsejtek képződését.
mechanizmus: vélhetőleg a topoizomeráz II enzimet gátolja → S fázis blokkolása → → nincs DNS replikáció (**DNS hibák**)
természetes forrása: Podophyllum növény, extrahálják a Podofillotoxint, amelynek származéka a **tenipozid**.

3. Pirrolvázás vegyületek

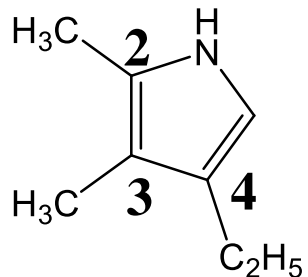
A. A pirrol szubsztituált származékai



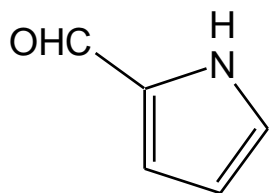
2-metilpirrol
2-Methylpyrrole



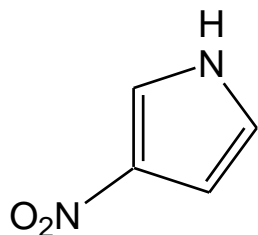
3-etil-4-metilpirrol
3-Ethyl-4-methylpyrrole



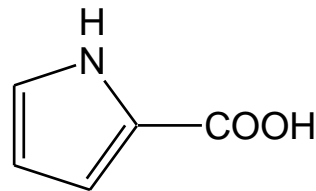
4-etil-2,3-dimetilpirrol
4-Ethyl-2,3-dimethylpyrrole



pirrol-2-karbaldehyd
Pyrrole-2-carbaldehyde

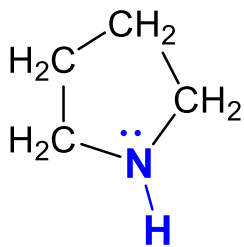


3-nitropirrol
3-Nitropyrrole

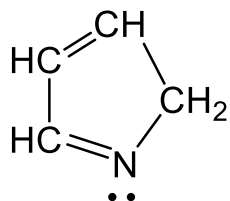


2-pirrolkarbonsav
Pyrrole-2-carboxylic acid

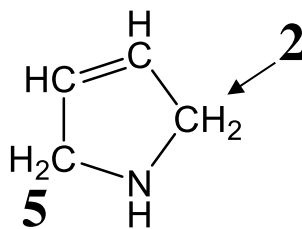
B. Telített pirrolszármazékok



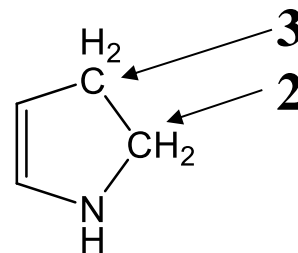
pirrolidin
Pyrrolidine



2H-pirrol
2H-Pyrrole



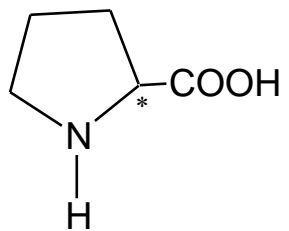
3-pirrolin
2,5-Dihydropyrrole



2-pirrolin
2,3-Dihydropyrrole

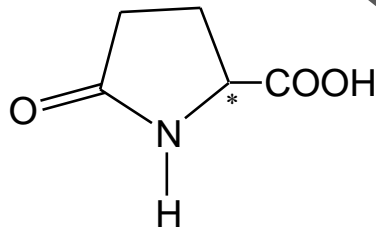
Érdekes pirrolidinszármazékok:

prolin



pirrolidin-2-karbonsav
Pyrrolidine-2-carboxylic acid

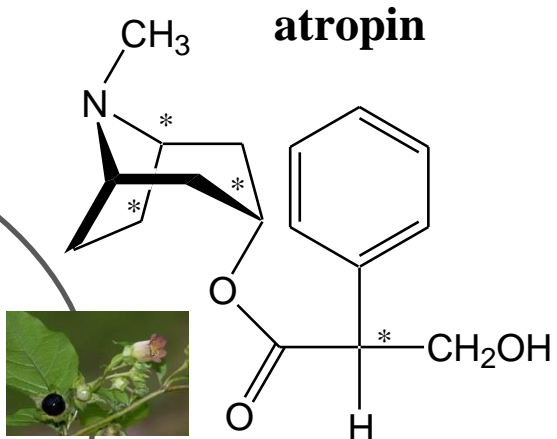
piroglutaminsav



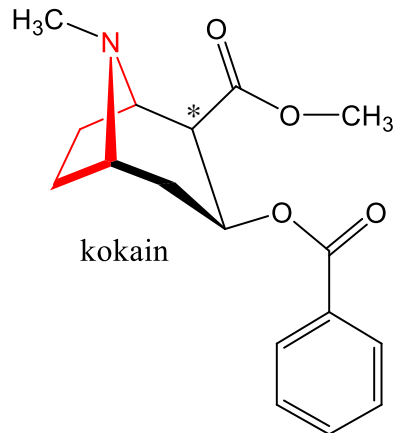
5-oxopirrolidin-2-karbonsav
5-Oxopyrrolidine-2-carboxylic acid

aminosavak

atropin



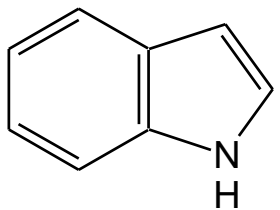
memo: tropánvázias alkaloid burgonyafélékből, nadragulyából izolálható erős mérge, acetilkolin recept. gátló
(*Atroposz* (görög) az a párka aki elvágja a halandó életfonalát)
+ szívgyógyszer (pl. bradycardia)



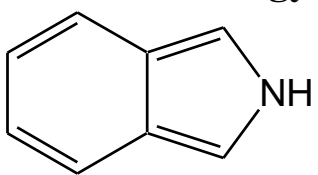
kokain



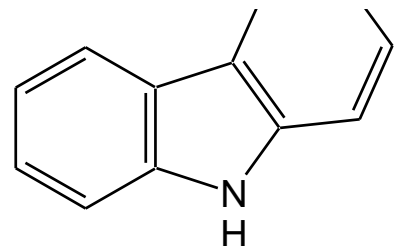
C. A pirrol benzológjai



indol
Indole
vagy: benzo[b]pirrol

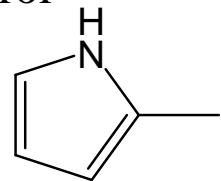


izoindol
isoindole

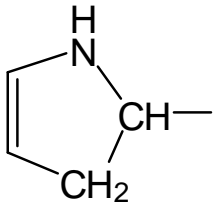


karbazol
vagy: dibenzopirrol

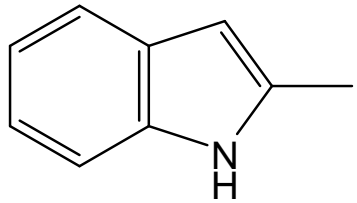
D. Csoportnevek



2-pirrolil-



(2-pirrolin)-5-il



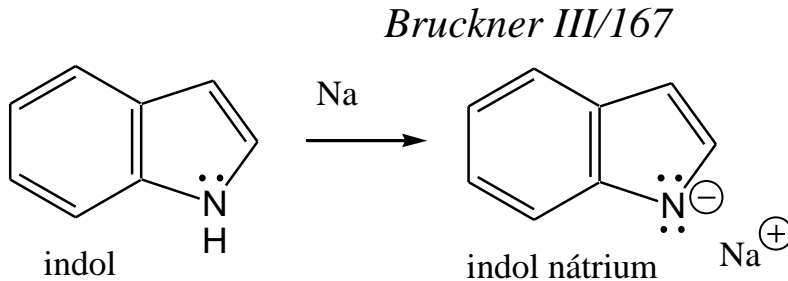
2-indolil-



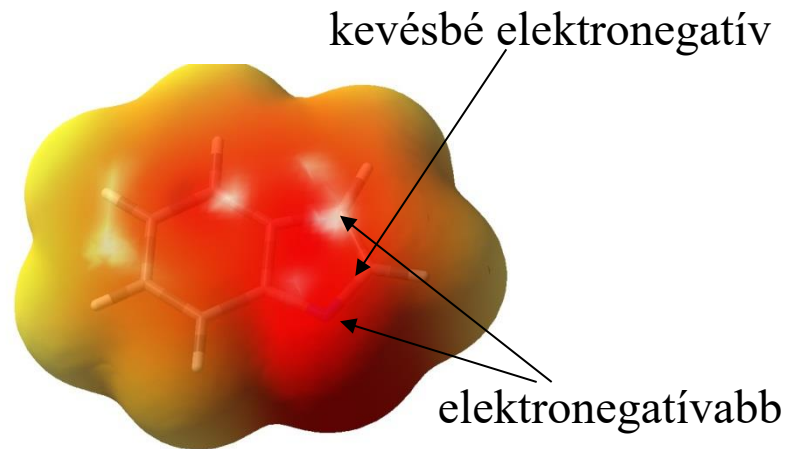
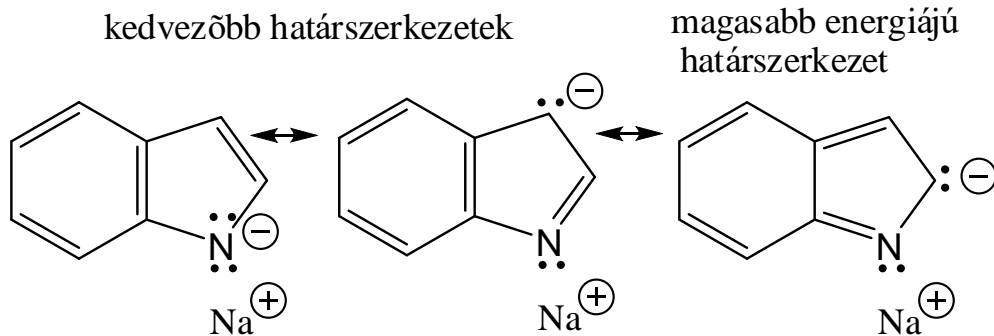
Koller (1884) a kokain kiváló helyi érzéstelenítő hatásáról számolt be.



memo: Az indol a pirolhoz hasonlóan „savas” karakterű:
 $pK_a=16.2$

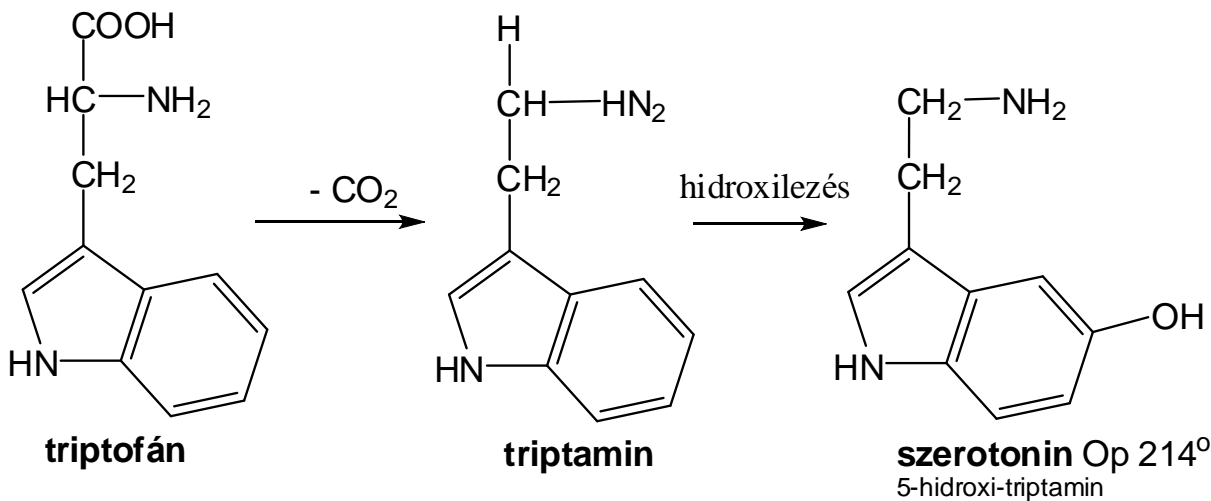


az indolát anion aromás jellege:



határszerkezetek a parciális polaritások értelmezéséhez

Példák fontosabb indolvázias vegyületekre:

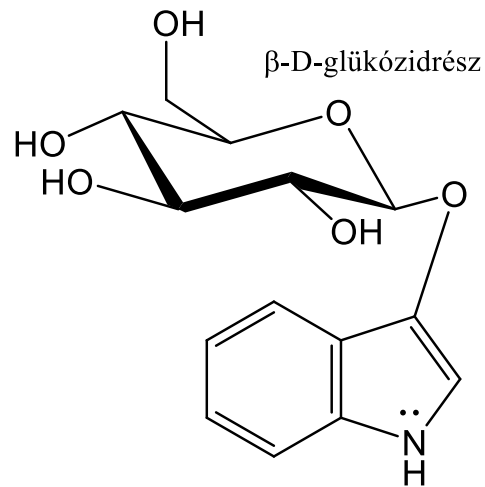


memo:

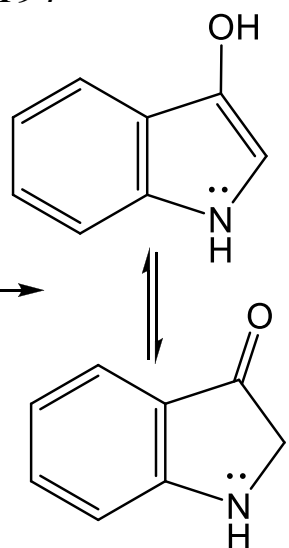
a szerotonin (lat. serum + gör. tonosz ‘feszített’) vérnyomás szabályzó (érösszehúzó), hormonhatású (melatonin prekursora), neurotranszmitter anyag

fluoreszkál : abszorpció: 280nm, emisszió (szolvatokróm): 300-350nm!

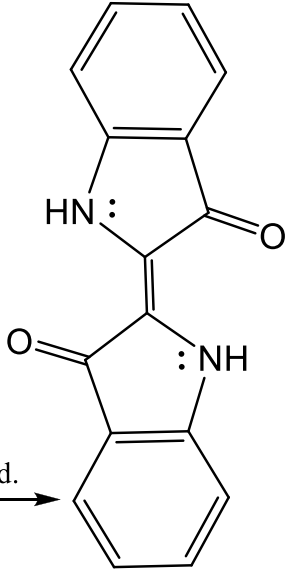
Bruckner III/194



savas hidrol.



oxid.



memo:
az indigó **kiterjedt konjugációs** rendszere felelős a színéért

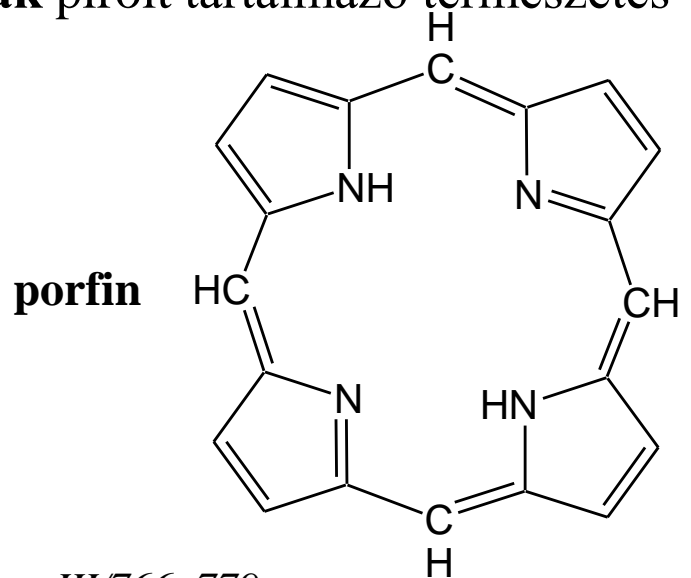
indikán op: 178°
β-D-glükózidil-indoxil
indigócserje, festőfű

indoxil
(két tautomerje)

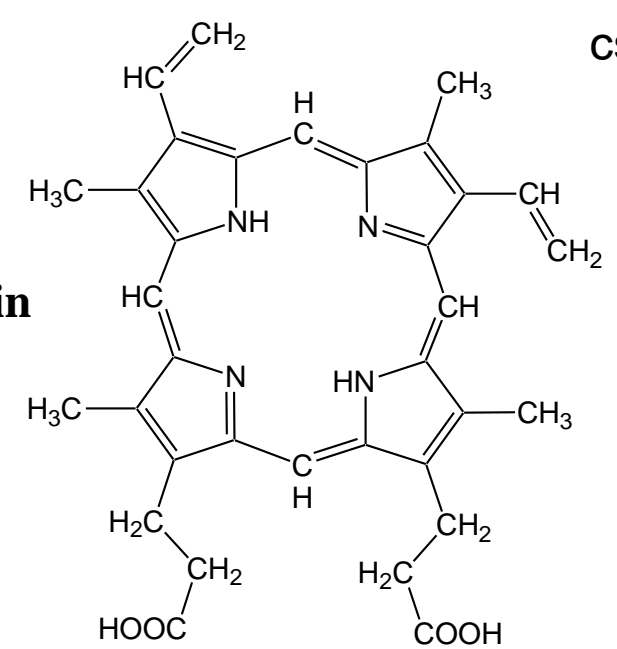
indigó Op 392°
csávaszinezék:
sötétkék



Példák pirolt tartalmazó természetes vegyületekre:

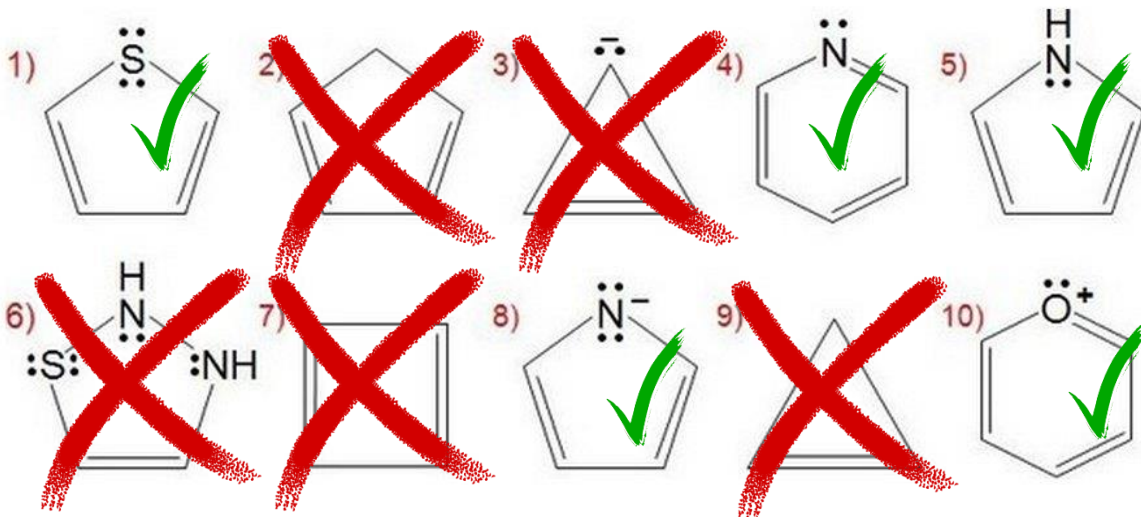
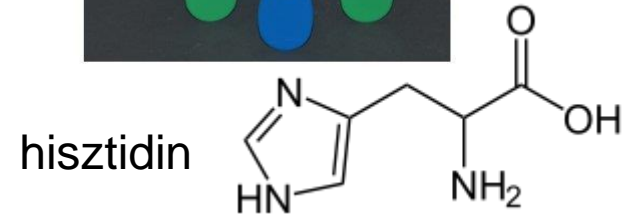
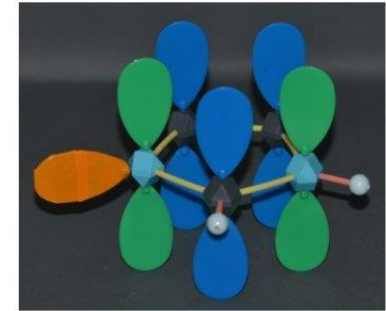
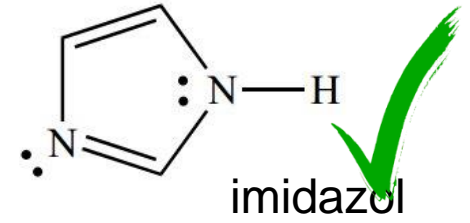
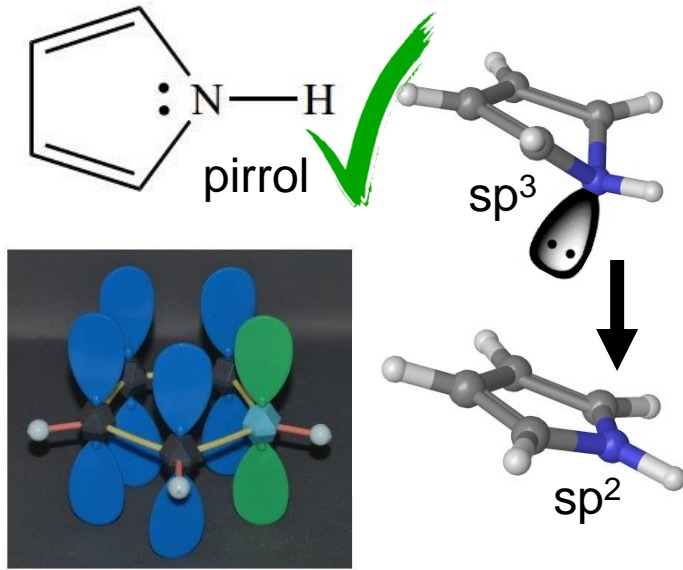
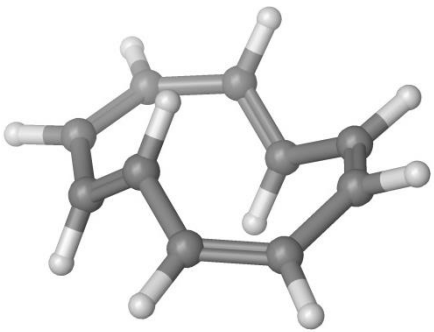
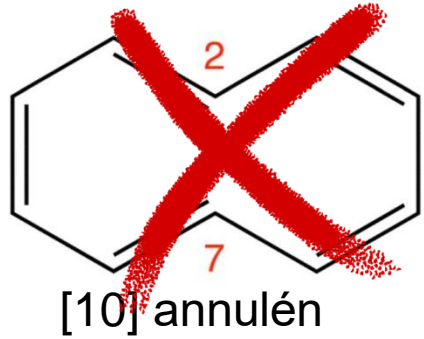


protoporfirin



Bruckner III/766, 779

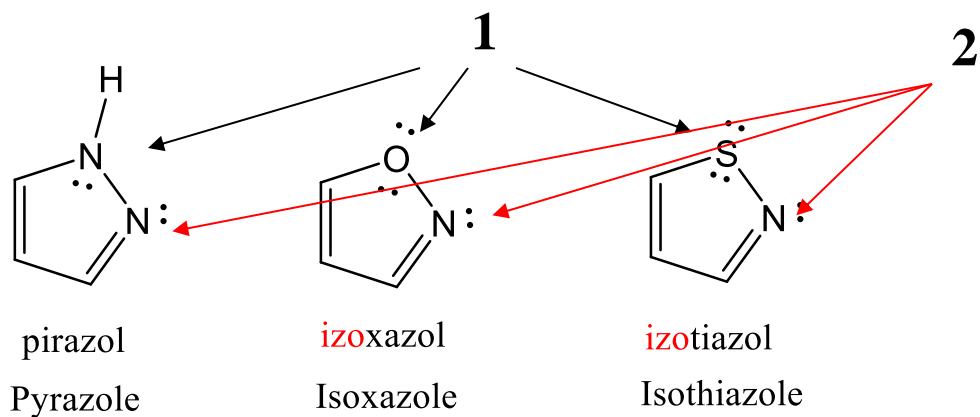
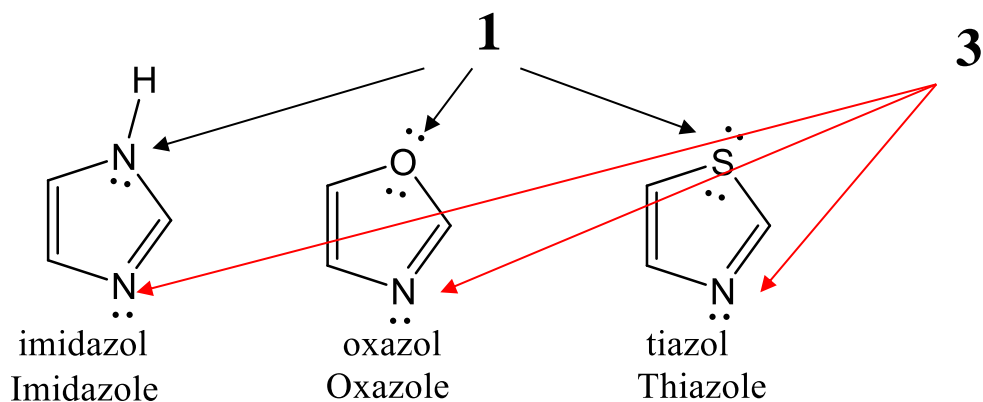
Aromás-e?



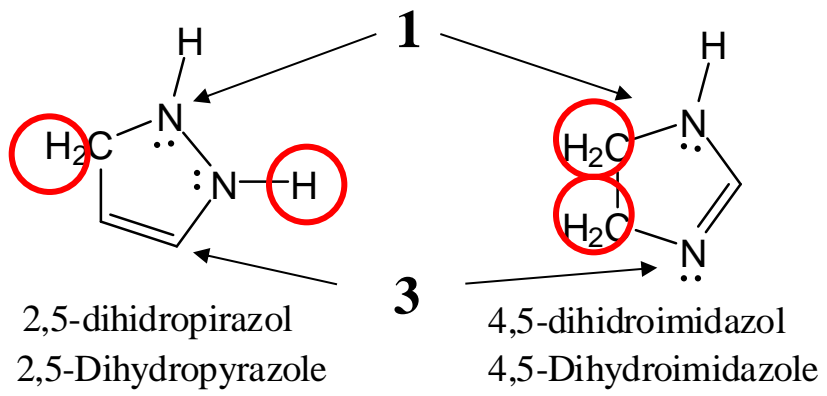
cikloheptatrienilium kation
(tropolium ion)

XVI. Heterociklusos szénvegyületek: két heteroatomos öttagú gyűrűk

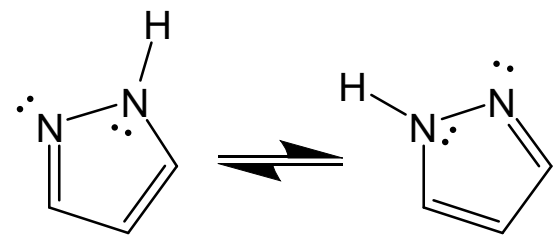
Azolok



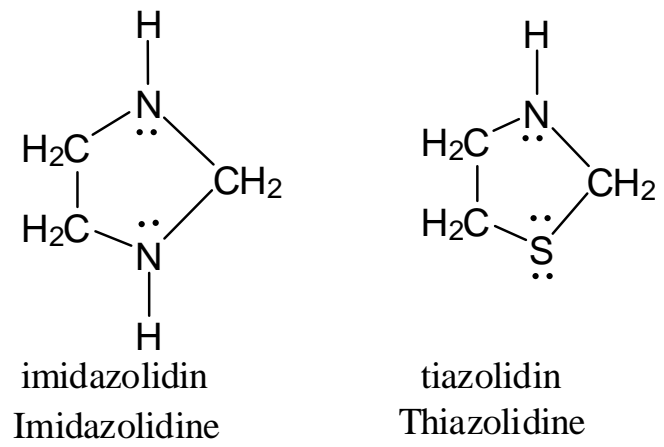
Azolinok



virtuális tautoméria:



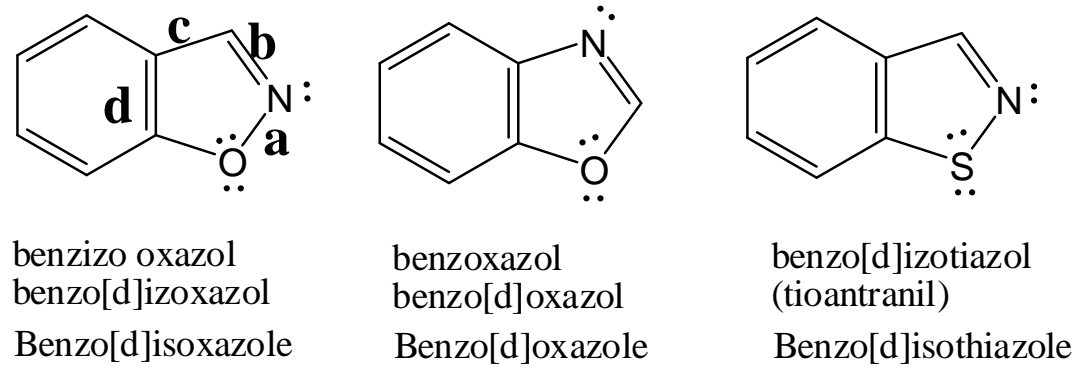
Azolidinek



Nevezéktan:

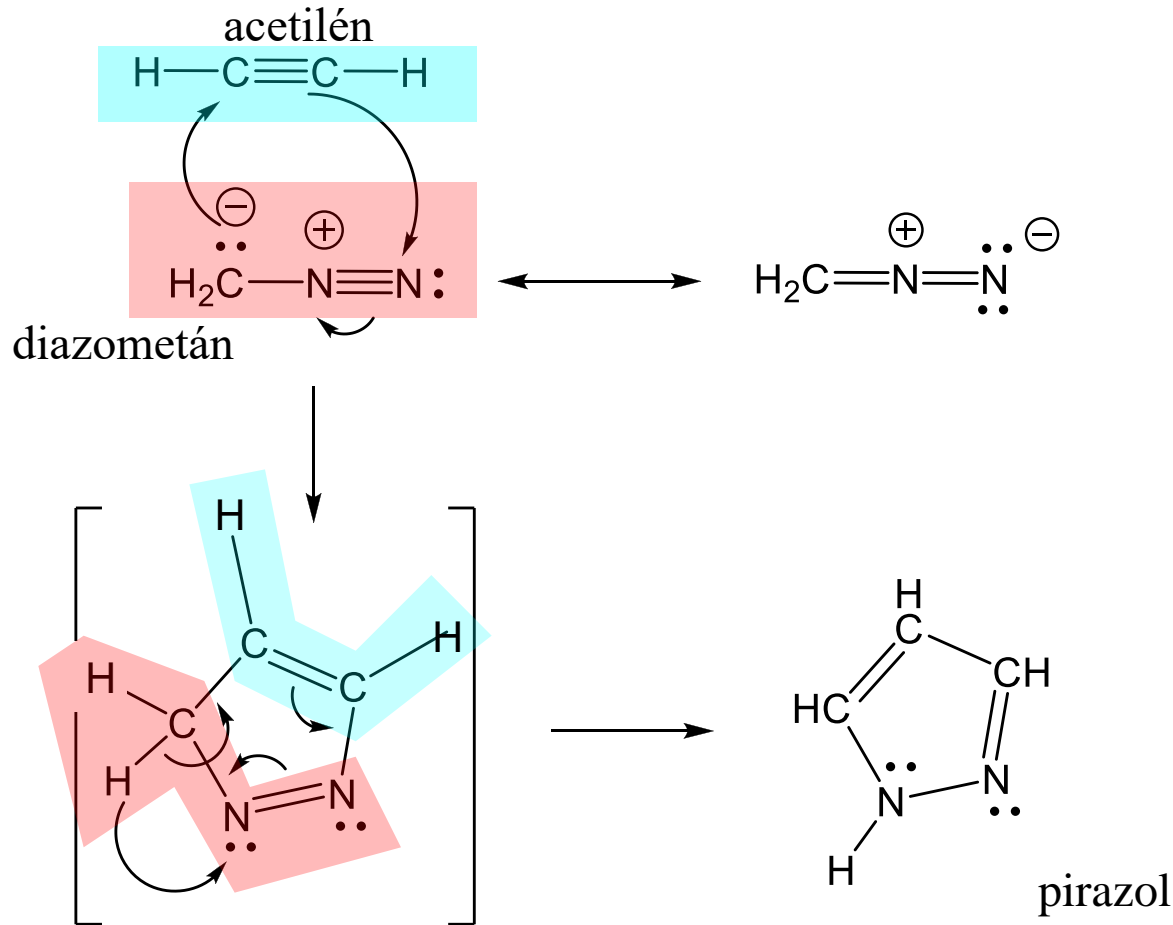
- azolok:** legalább egy N-t tartalmaz a gyűrű
- azolinok:** az azolok dihidroszármazékai
- azolidinek:** az azolok tetrahidroszármazékai

Benzológok



példa: a pirazol (egy két heteroatomot tartalmazó öttagú heterociklusos vegyület) szintézisére

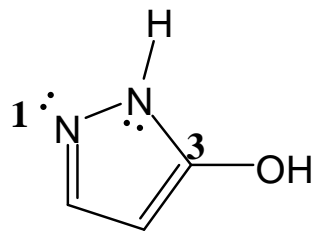
memo: a diazometán, mint nukleofil szerepel egy nukleofil addíciós reakcióban, éterben oldva laboratóriumi körülmények közt használható (szabad gáz robbanékony))



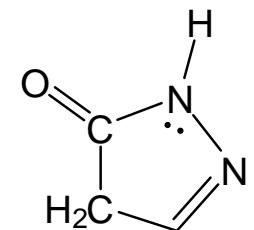
memo2: a diazometán megfelelő határszerkezetével értelmezzük a reakciót

megvalósítás:
(Pechmann 1898)
A diazometán éteres oldatát hűtjük és ebbe vezetjük be az acetiléngázt

1. Pirazolvázás vegyületek

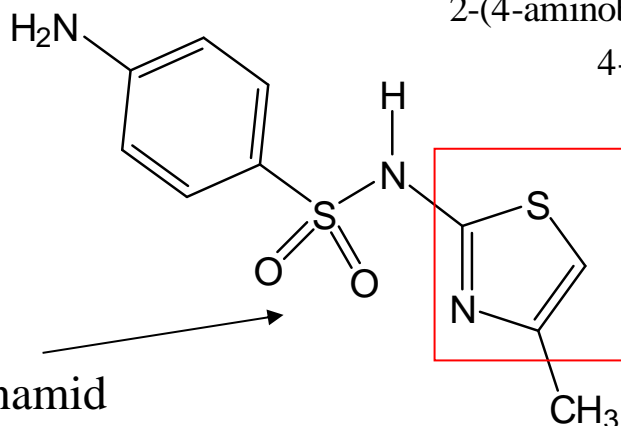


2H-pirazol-3-ol
2H-Pyrazol-3-ol



4,5-dihidropirazol-5-on
4,5-Dihydropyrazol-5-one

2. Tiazolvázás vegyületek



2-(4-aminobenzolszulfonamido)-4-metiltiazol
4-Amino-N-(4-methyl-2-thiazolyl)-
benzenesulfonamide

Ultraseptyl
kiváló baktericid hatását
(Chinoin 1939-től)

szulfonamid

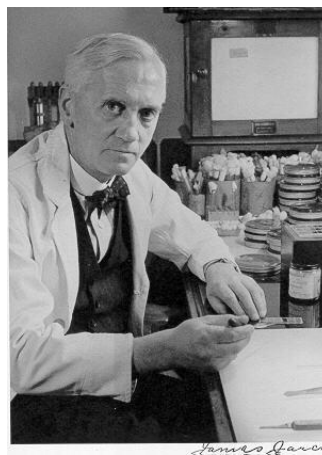
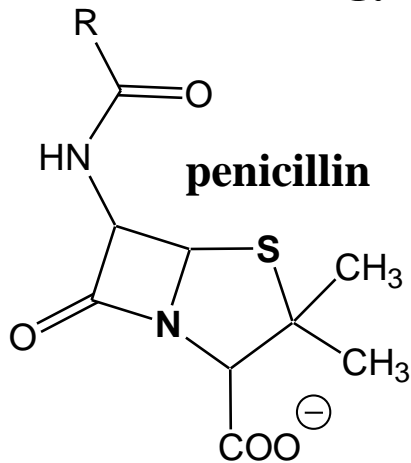
Az antibakteriális Ultraseptyl előállítása

1939

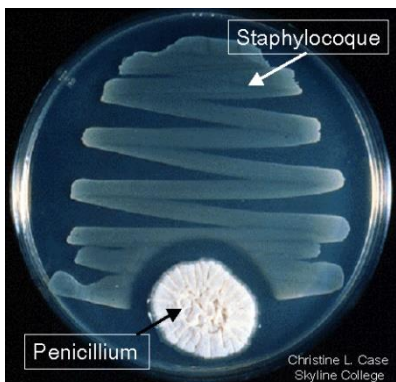
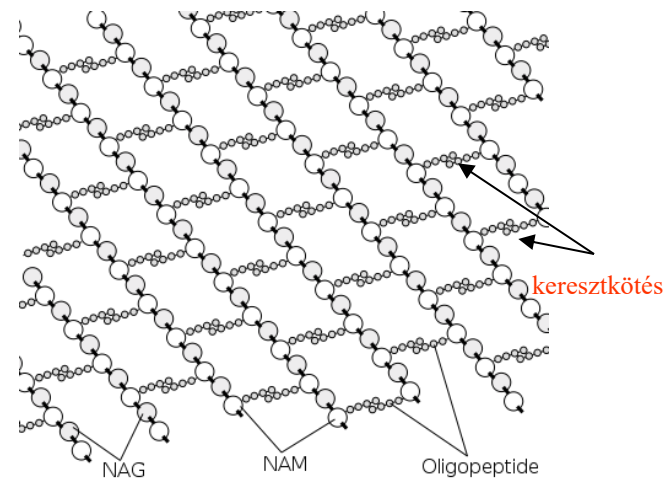
1939-ben áttörő sikert ért el a Chinoin az antibakteriális Ultraseptyl előállításával, melyet Dr. Wolf Emil, Dr. Földi Zoltán, Gerecs Árpád és König Rezső dolgozott ki. A vizsgálatok során az Ultraseptyl bizonyult a leghatásosabb és a legkevesebb mellékhatással rendelkező készítménynek. Ezek után a II. Világháborúban a harcoló felek között nagyon elterjedt a készítmény. A németeken és a szövetségeseken kívül az Ultraseptyl eljutott a semleges Törökországon keresztül az angol hadseregbe, az USA-ba, sőt a Szovjetunióba is. 1945-ben orosz katonák is az ismert gyógyszert keresték a gyárban.



Példák tiazolidin gyűrűt tartalmazó természetes vegyületre:



Alexander Fleming
(1881-1955)

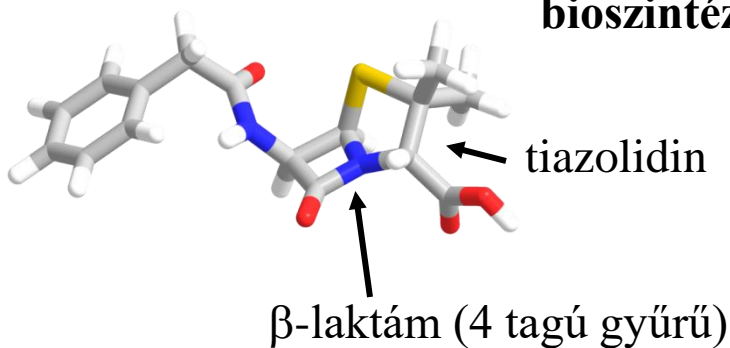


megfigyelés: a *Staphylococcus* baktérium kultúrájának a növekedését gátolja a *Penicillium notatum* gomba anyagcseréjének terméke, a penicillin.

hatáskeresztmetszet:

általában a Gram+ baktériumokra hat. a sejtfalokban található peptidoglikánokra jellemző **kereszt-kötésének** kialakulását gátolja (transzpeptidáz inhibitora).

bioszintézis: cisztein, valin és L-amino-adipinsav szükséges

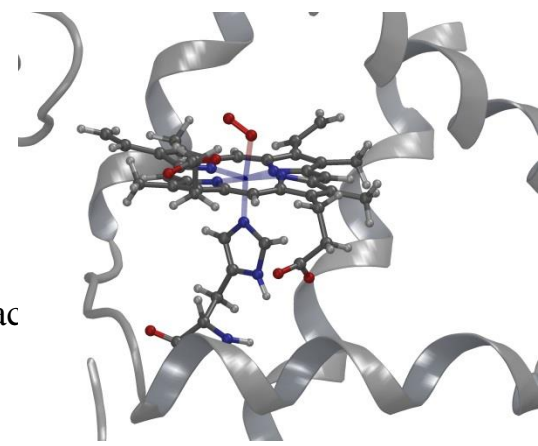
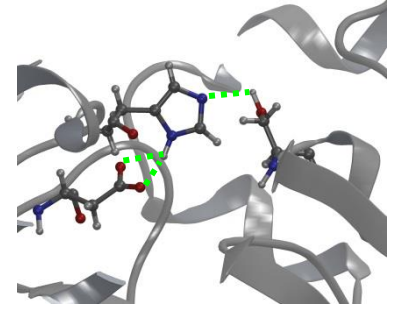
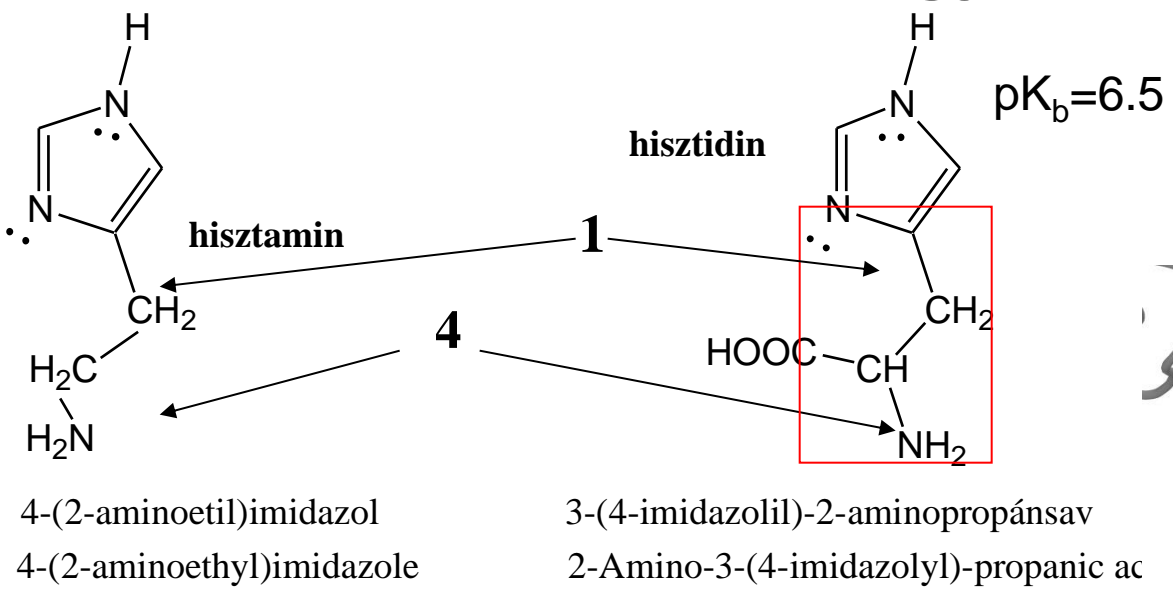


D-Ala-D-Ala részletre hasonlít \rightarrow enzim Ser oldalláncához kötődik kovalensen

3. Imidazolvázas vegyületek



ANYARÓZS
(CLAVICEPS PURPUREA)

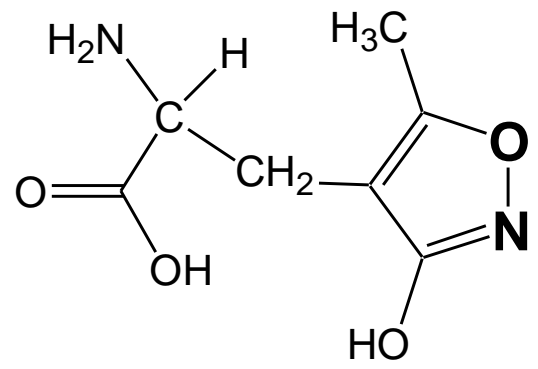


AMPA

hisztamin: az anyarózs, egy növényi kórokozó gomba, alkaloidja, a varangyméreg egyik komponense –
Immunreakció (simaizom-serkentés, fájdalom/viszketés-érzet), ébrenlét-alvási ciklus szabályozása, bélműködés reguláció....

Egy példák izooxazol gyűrűt
 tartalmazó természetes vegyületre:

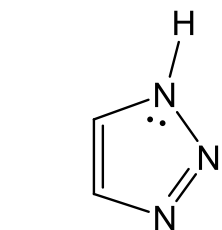
Az AMPA egy **glutamát receptor (AMPA) agonistája**
 Glutamát: fontos szerepe van a szinapszisokban történő neurotranszmisszióban, a tanulási folyamatok kialakulásában
memo: a glutamát nagy mennyiségben idegrendszeri betegségekhez vezethet



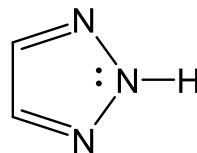
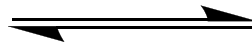
alpha-amino-3-hydroxy-5-methyl-4-isoxazole propionic acid

XVII. Heterociklusos szénvegyületek: több-heteroatomos öttagú gyűrűk

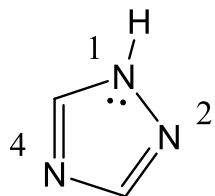
Tautomerek egyensúlyi rendszere



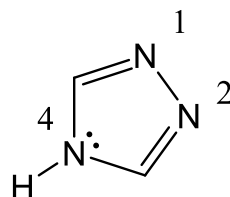
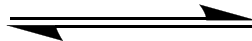
1,2,3-triazol
1,2,3-Triazole



2H-1,2,3-triazol
2H-[1,2,3]Triazole

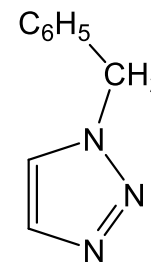


1H-[1,2,4]-triazol
1H-[1,2,4]Triazole

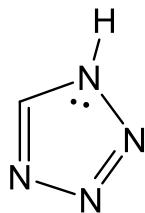


4H-[1,2,4]-triazol
4H-[1,2,4]-Triazole

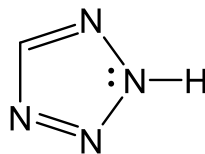
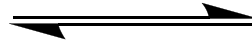
Nev. gyak.:



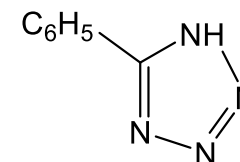
1-benzil-1,2,3-triazol
1-Benzyl-1,2,3-triazole



tetrazol
Tetrazole



2H-tetrazol
2H-Tetrazole

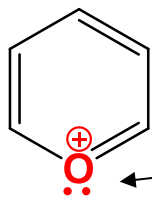


5-fenil-tetrazol
5-Phenyl-tetrazole

XVIII. Heterociklusos szénvegyületek: egy heteroatomos hattagú gyűrűk (Bruk. III/1 338.)

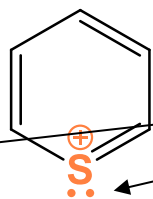
Aromás vegyületek

oxónium kation

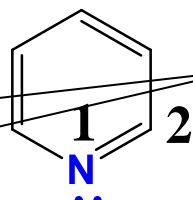


pirilium kation
Pyrilium cation

szulfónium kation



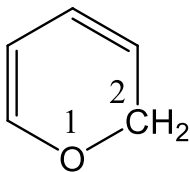
tiapirilium kation
Thiapyrylium cation



piridin
Pyridine

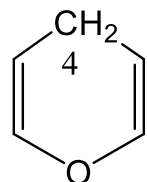
Pozitív töltés mivel az egyik nemkötő elektronpárjuk részt vesz a közös π -rendszerben.

Nem aromás származékok



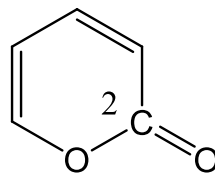
2H-pirán
(α -pirán)

2H-Pyran

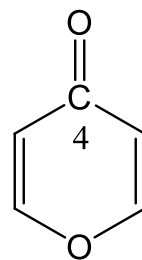


4H-pirán
(γ -pirán)

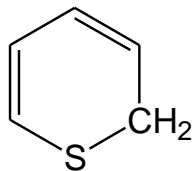
4H-Pyran



2H-pirán-2-on
(α -piron)

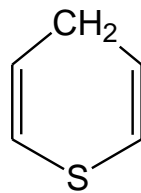


4H-pirán-4-on
(γ -piron)



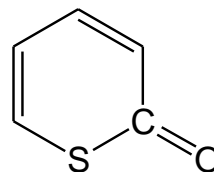
2H-tiopirán
(α -tiopirán)

2H-Thiopyran



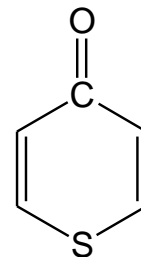
4H-tiopirán
(γ -tiopirán)

4H-Thiopyran



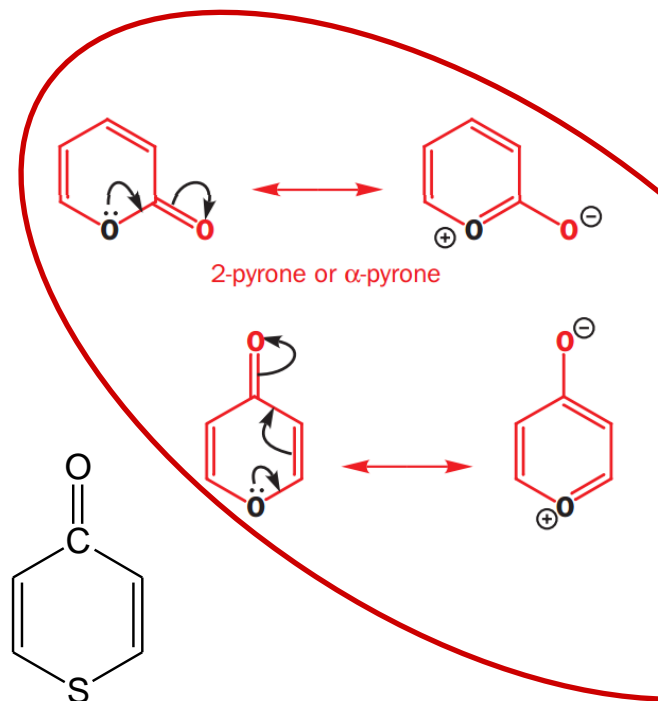
2H-tiopirán-2-on
(α -tiopiron)

Thiopyran-2-one



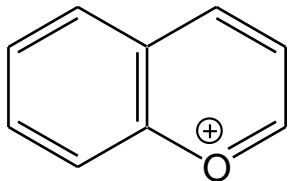
4H-tiopirán-4-on
(γ -tiopiron)

Thiopyran-4-one

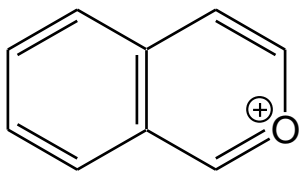


1. Piránok benzológjai

Aromás vegyületek:

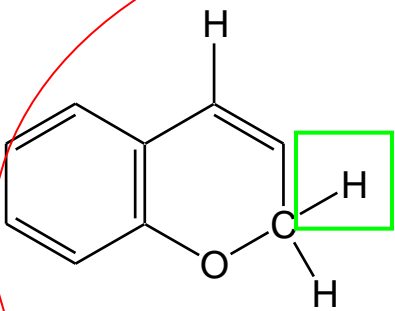


benzpirilium kation

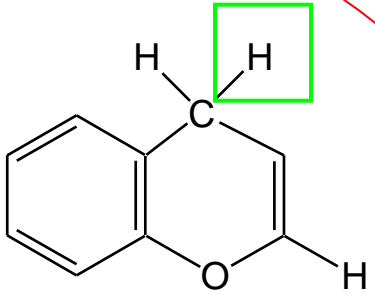


izobenzpirilium kation

Nem aromás származékok:

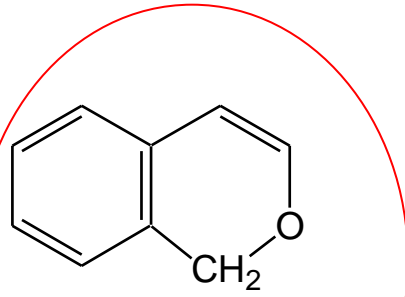


2H-kromén
(α -kromén)
2H-Chromene



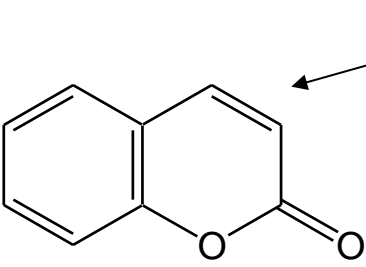
4H-kromén
(β -kromén)
4H-Chromene

tautomerek

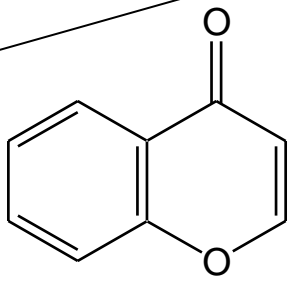


izokromén
1H-Ischromene

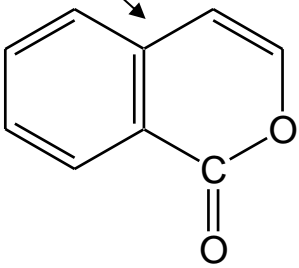
konstitúciós izomerek



kumarin
Chromen-2-one



kromon
Chromen-4-one



izokumarin
Isochromen-1-one

Természetes vegyületek oxigén-heteroatommal:

Bruckner III-414

flavonoidok

(*flavus* = sárga [latin])

-OH-t és fenilcsoportot tartalmazó

kromon jellegű molekulák,

amelyek

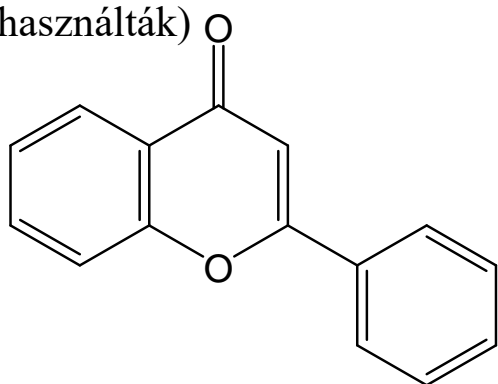
gyakran glikozilezettek,

virágszirmok

színezékei

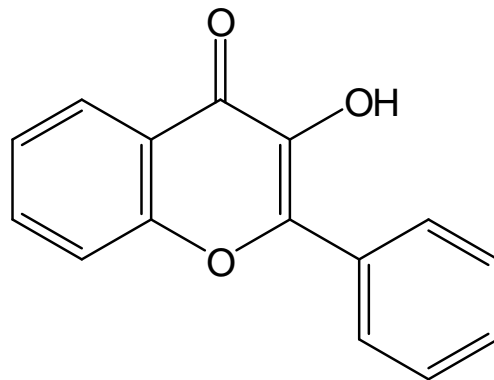
(sárga textil színezékként

használták)



2-fenilkromán-4-on
(flavon)

2-Phenylchroman-4-one

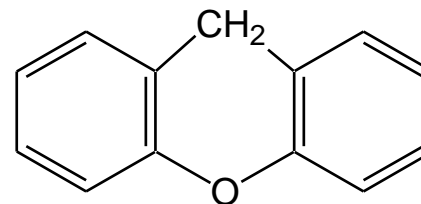


2-fenil-3-hidroxikromá-4-on
(flavonol)

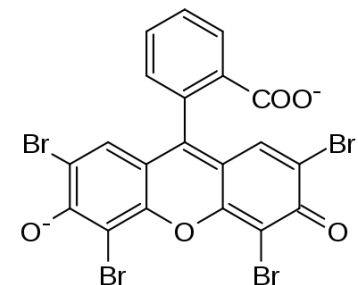
3-Hydroxy-2-phenylchroman-4-one



Xantének (dibenzopiránok) -festékek



xantén
Xanthene

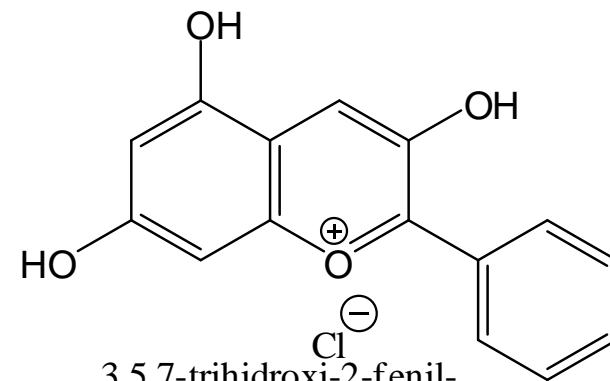


Eozin: izom/kollagén megfestése

antocianidinek

virágszirmok , gyümölcshéjak

pigmentjeinek színezékei (piros, bíbor, ibolya etc.)



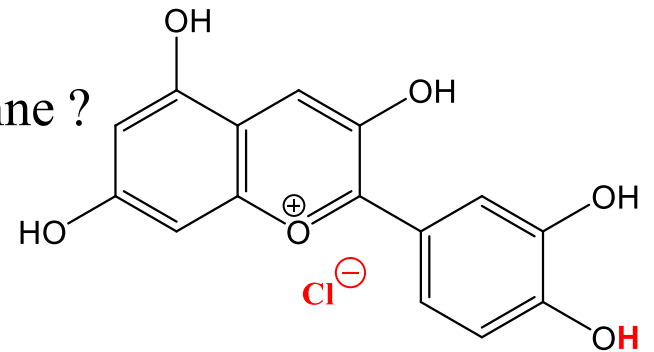
3,5,7-trihidroxi-2-fenil-
benzopiriliium-klorid
(3,5,7-trihidroxiflavilium-klorid)

3,5,7-Trihydroxy-2-phenyl-
benzopyryliumchloride

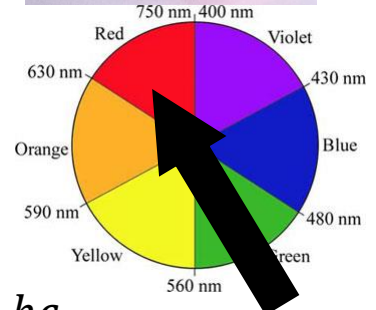
kérdés: mitől piros a rózsza és mitől kék a búzavirág holott ugyanaz az antocianidin rész van benne ?



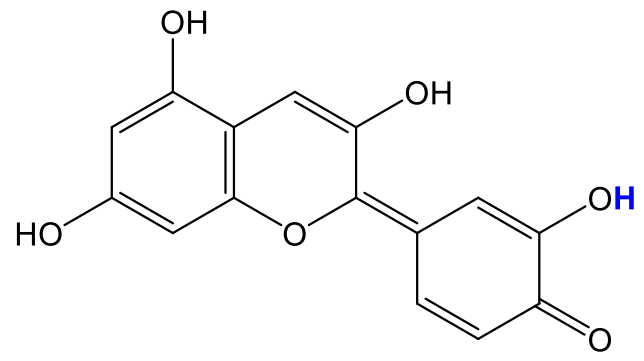
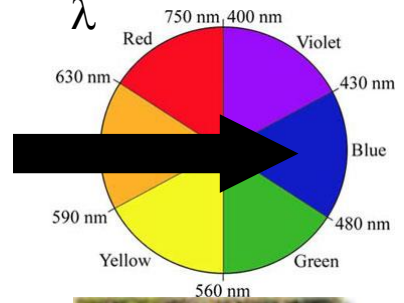
**pH=3
vörös szín (rózsza)**



2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-chromenylium chloride



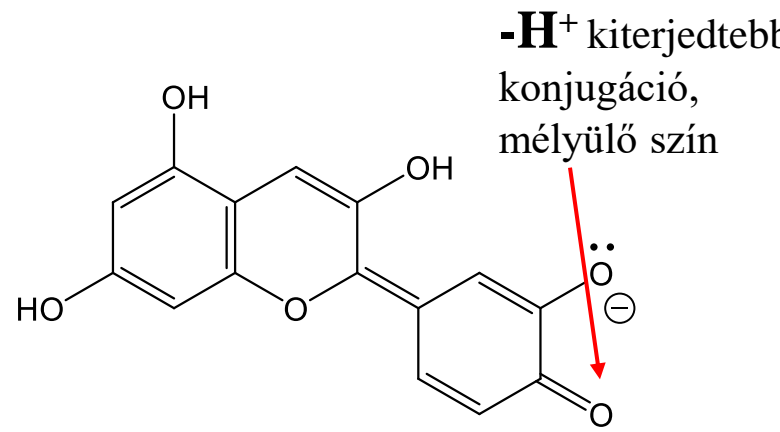
$$E = hv = \frac{hc}{\lambda}$$



2-Hydroxy-4-(3,5,7-trihydroxychromen-2-ylidene)-cyclohexa-2,5-dien-1-one



**pH=8
kék szín (búzavirág)**



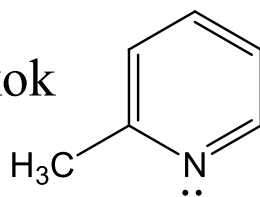
2-Oxo-3-(3,5,7-trihydroxy-chromen-2-ylidene)-cyclohexa-1,4-dienol anion

válasz:
a konjugáció kiterjedésének nagysága eltérő

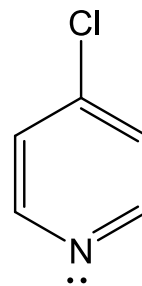
2. Piridin és származékai

A. A piridin szubsztituált származékai:

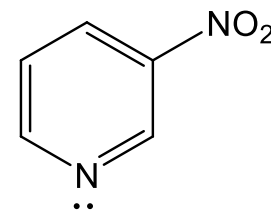
Monoszubsztituált származékok



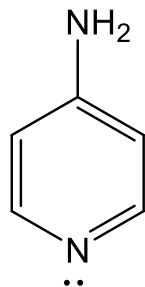
2-metilpiridin
(2-pikolin, α -pikolin)
2-Methylpyridine



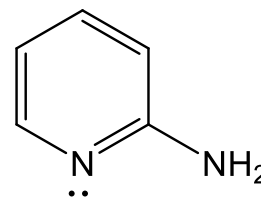
4-klórpíridin
4-Chloropyridine



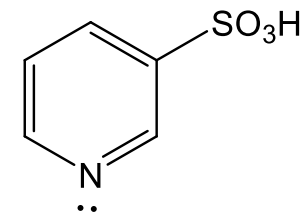
3-nitropíridin
3-Nitropyridine



piridin-4-amin
Pyridine-4-amine

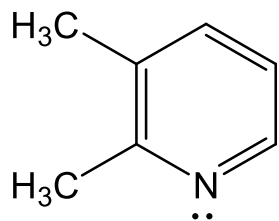


piridin-2-amin
Pyridine-2-amine

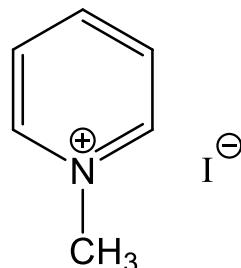


piridin-3-szulfonsav
Pyridine-3-sulfonic acid

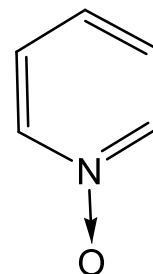
Diszubsztituált származékok, oxidok és sók



2,3-dimetilpiridin
2,3-Dimethylpyridine

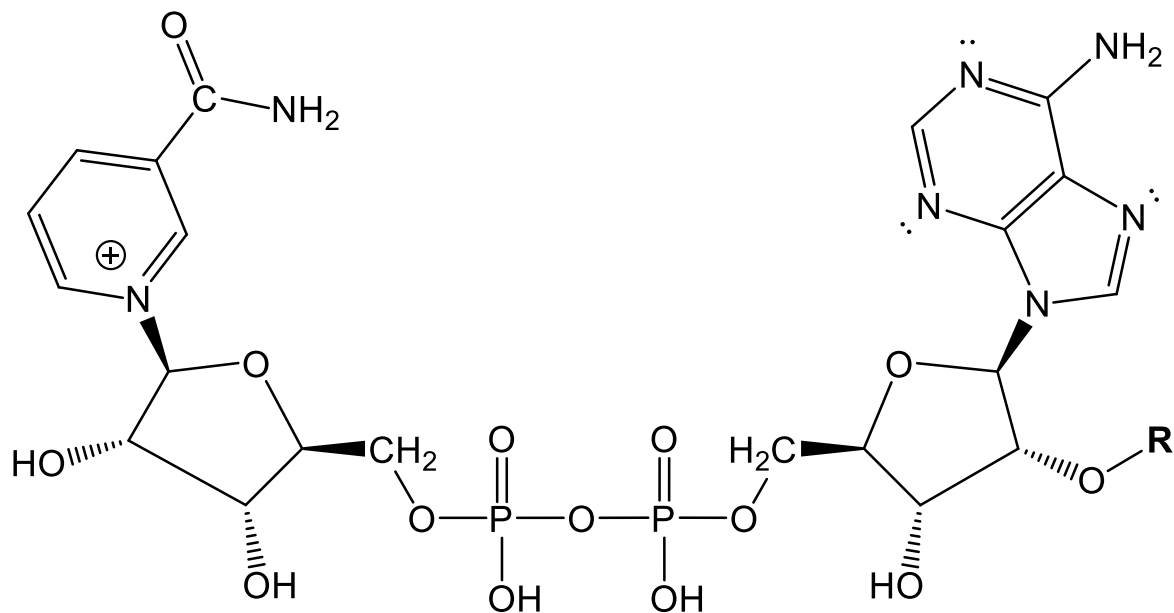


N-metilpiridinium-jodid
1-Methylpyridinium iodide



piridin-N-oxid
Pyridine 1-oxide

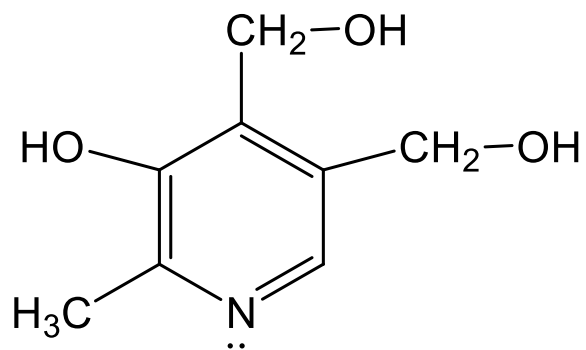
Piridint tartalmazó fontos természetes vegyületek:



Nikotinamid-adenin-dinukleotid (oxidált forma)

R=H: NAD, **R**=PO₃²⁻: NADP

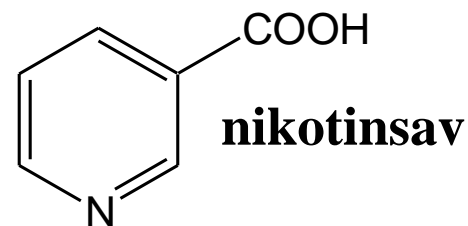
[Stryer 449]



Piridoxin

[Stryer 631]

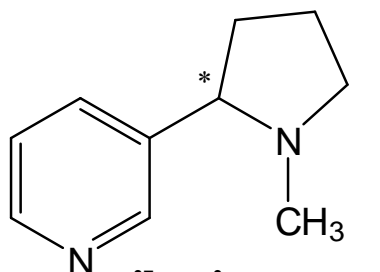
(B₆ vitamin)



piridin-3-karbonsav
pyridine-3-carboxylic acid

Dohányalkaloidok:

Bruckner III/892

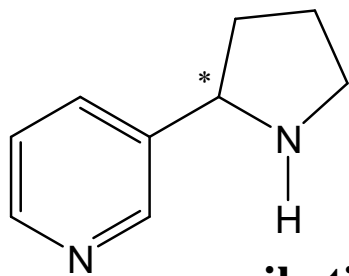


nikotin fp 246°

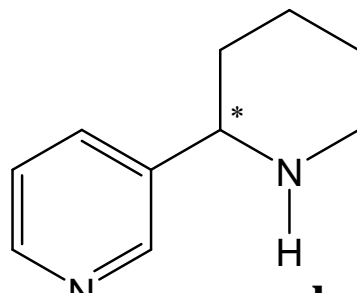
szintelen olaj

a *Nicotina tabacum*

fő alkaloidja (75%)



nornikotin



anabazin

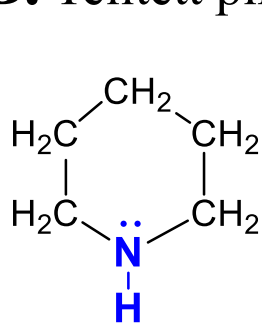


A nikotin **fiziológiás hatása**: erős idegméreg
továbbá: erős inszekticid (növényvédelem)

piridin-pirrolidin

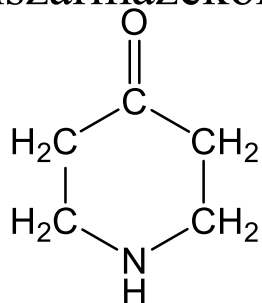
piridin-piperidin

B. Telített piridinszármazékok



piperidin

Piperidine

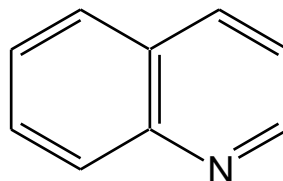


4-piperidon

Piperidine-4-one

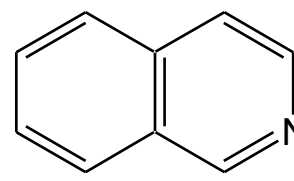


C. A piridin benzológjai



kinolin

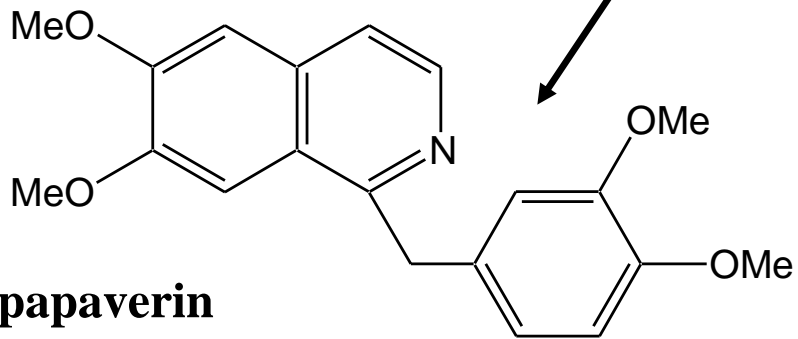
Quinoline



izokinolin

Isoquinoline

Ópium- vagy mákalkaloidok: I + II

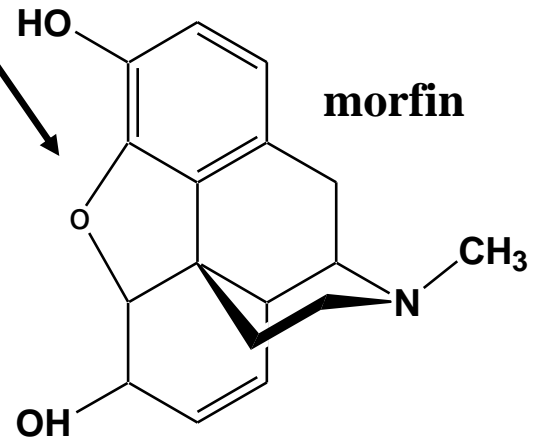


papaverin

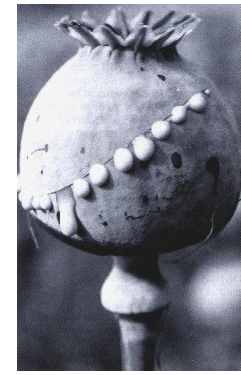
tipikus 1-benzil-izokinolinvázas alkaloid

benzo[c]piridin

Bruckner III/924



morfin

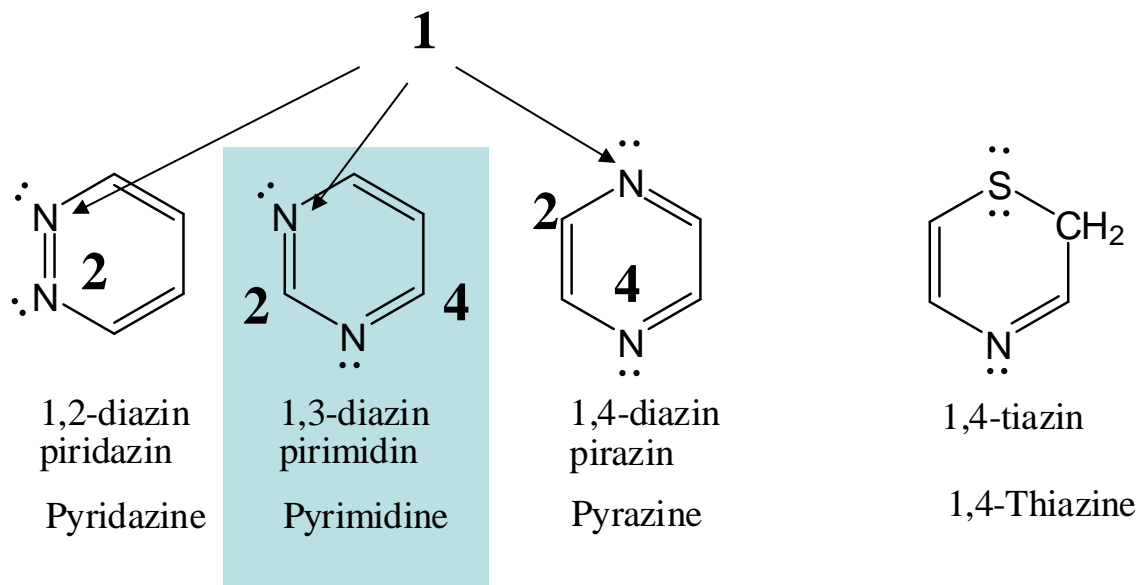


Az ópium **fiziológiás hatása**: fájdalomcsillapító és görcsoldó

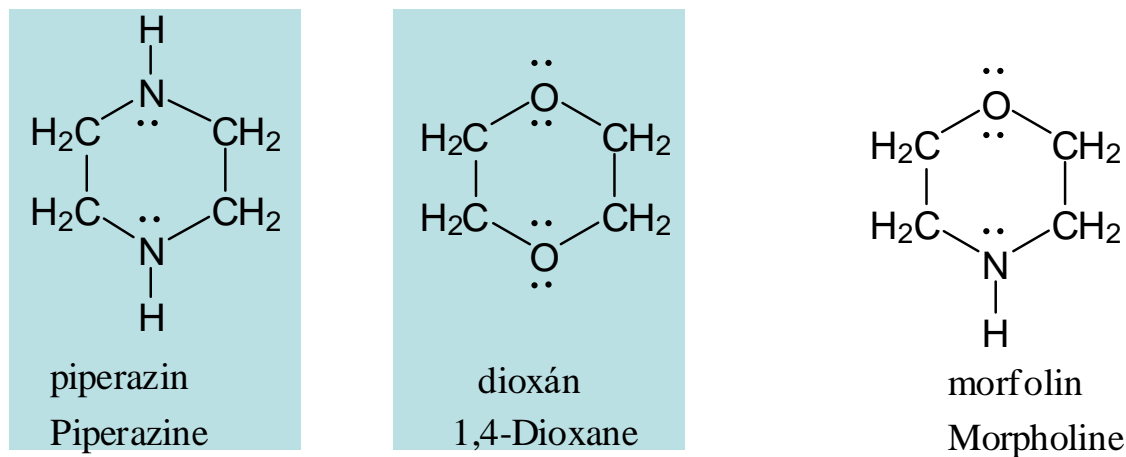
XIX. Heterociklusos szénvegyületek:

Két heteroatomos hattagú gyűrűk (Bruk. III/1 .)

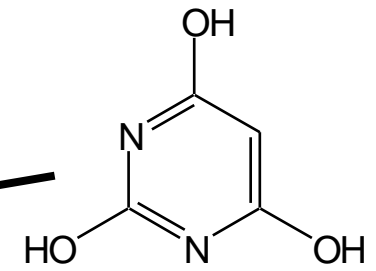
Aromás vegyületek:



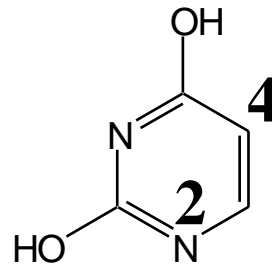
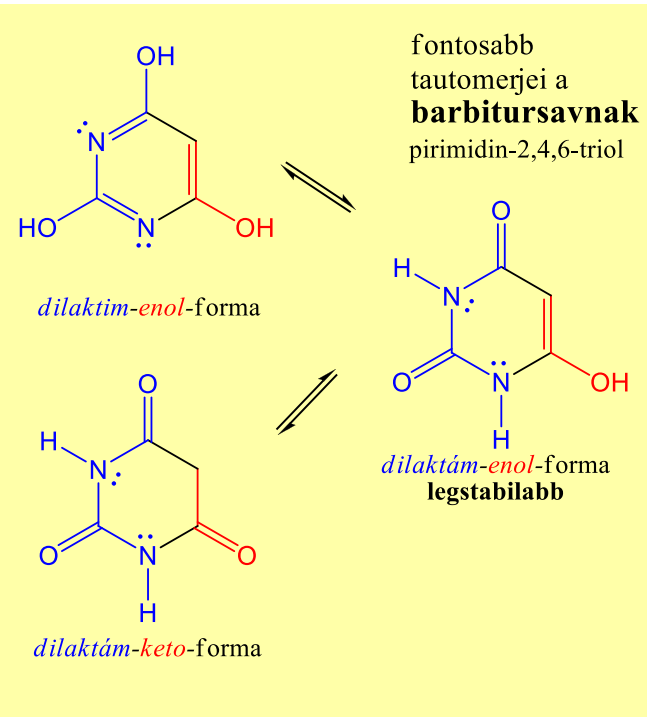
Nem aromás származékok:



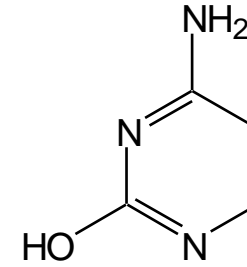
Pirimidinszármazékok



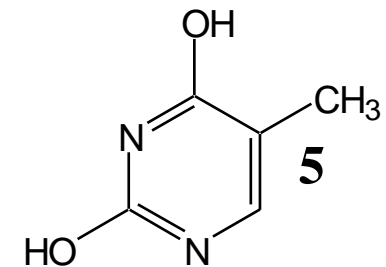
barbitursav
pirimidin-2,4,6-triol



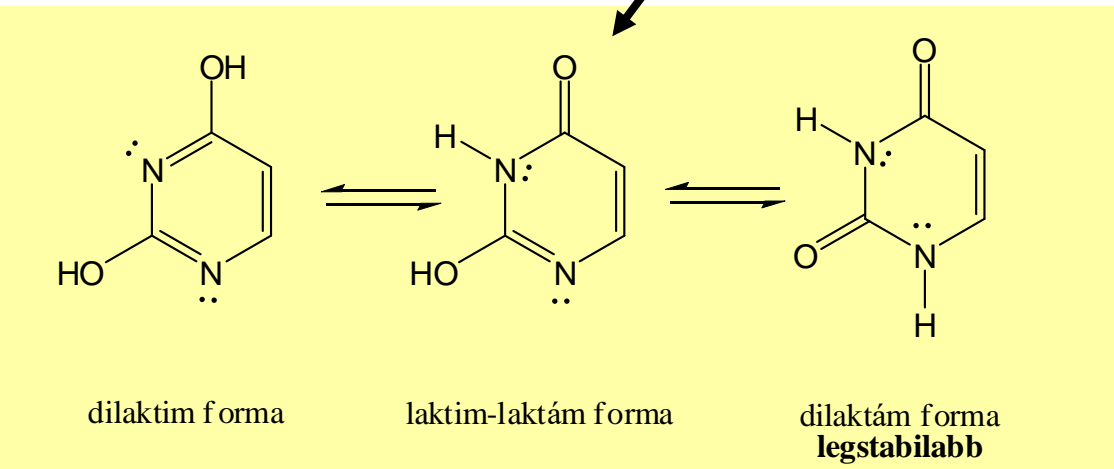
uracil
pirimidin-2,4-diol



citozin
4-amino-pirimidine-2-ol

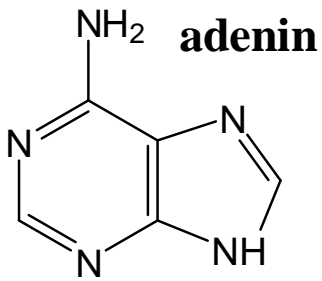


timin
5-metil-uracil
5-methyl-pyrimidine-2,4-diol

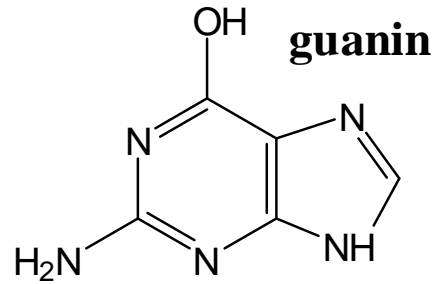


XX. Heterociklusos szénvegyületek több heteroatommal

Purinszármazékok

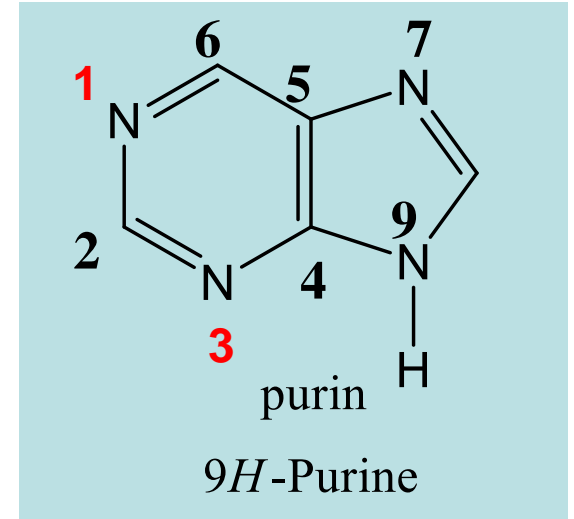


6-amino-purin
9H-Purine-6-ylamine
9H-purin-6-ilamin

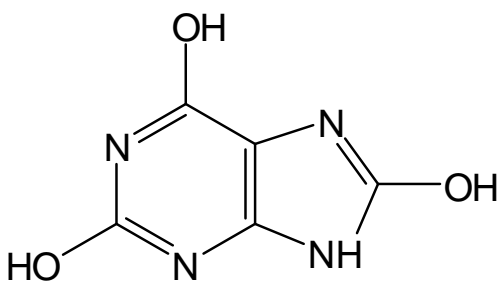


2-amino-6-hidroxi-purin
2-Amino-9H-purine-6-ol
2-amino-9H-purin-6-ol

Szn

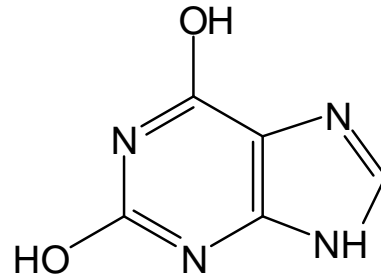


Példa purinvázis vegyületekre:



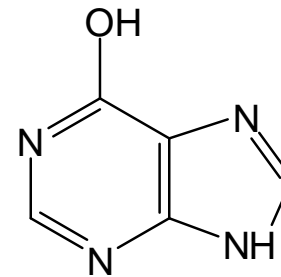
2,6,8-trihidroxi-purin

9H-Purine-2,6,8-triol
9H-purin-2,6,8-triol



2,6-dihidroxi-purin

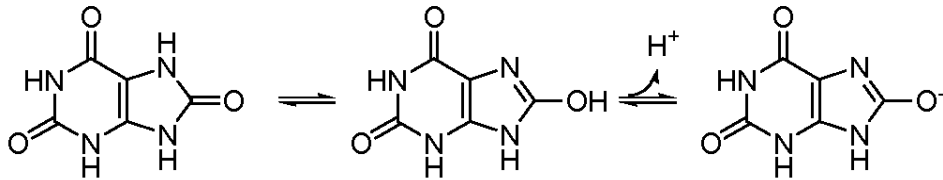
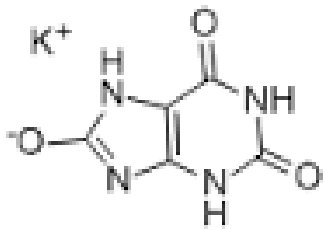
9H-Purine-2,6-diol
9H-purin-2,6-diol



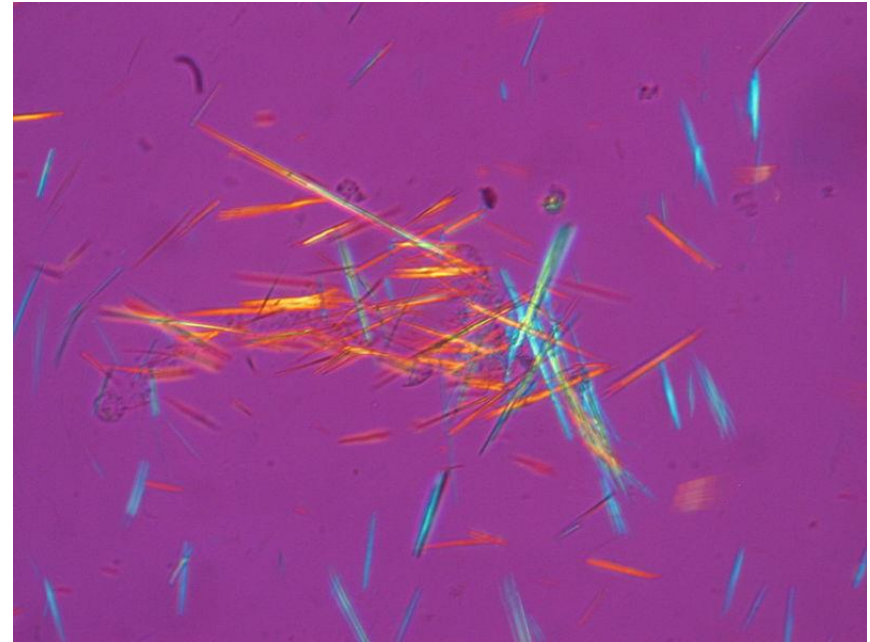
6-hidroxi-purin

9H-Purine-6-ol
9H-purin-6-ol

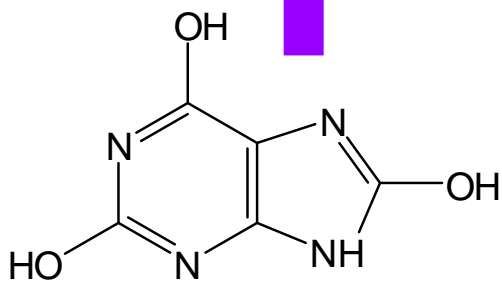
Szn



$pK_a = 5.6, 8.4$



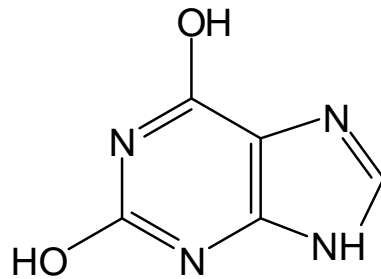
Példa purinvesztás vegyületekre:



hugysav

2,6,8-trihidroxipurin

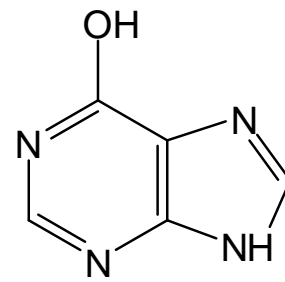
9H-Purine-2,6,8-triol
9H-purin-2,6,8-triol



xantin

2,6-dihidroxipurin

9H-Purine-2,6-diol
9H-purin-2,6-diol

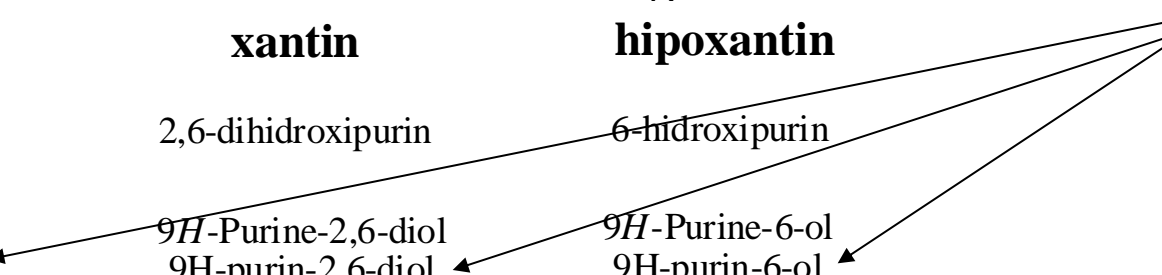


hipoxantin

6-hidroxipurin

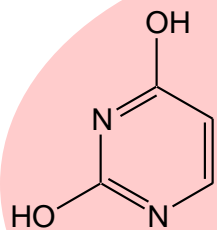
9H-Purine-6-ol
9H-purin-6-ol

Szn



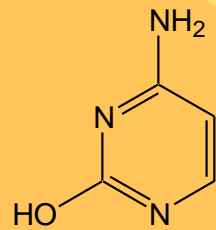
A nukleinsavak építőelemei:

heterociklusok (nukleo-bázisok):



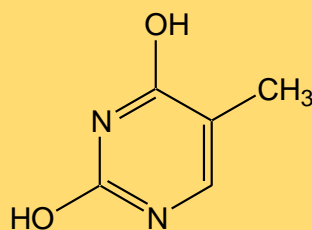
uracil

pirimidin-2,4-diol



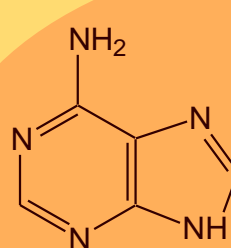
citozin

4-amino-pirimidine-2-ol



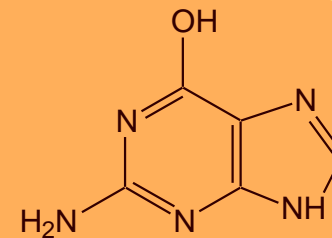
timin

5-methyl-pyrimidine-2,4-diol



6-amino-purin

adenin

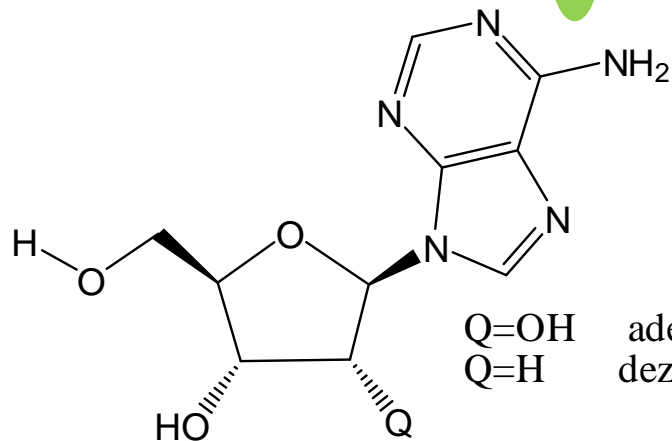


2-amino-6-hidroxi-purin

guanin

+ cukor (ribóz) :

● DNS
● RNS



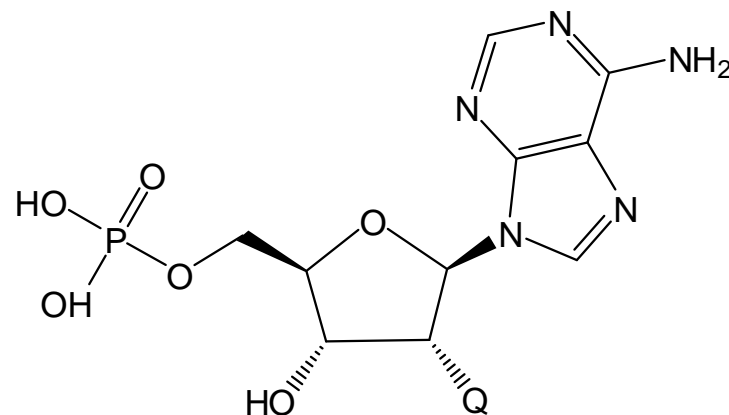
Q=OH
Q=H

adenozin
deziadenozin

Nukleozidok:

A megfelelő purin- és pirimidinbázisok N-glikozidjai

+ foszforsav :

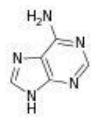
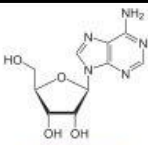
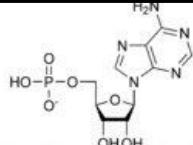
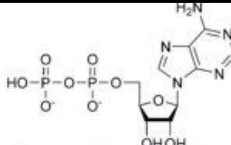
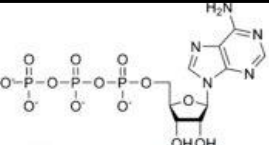
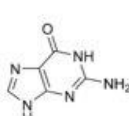
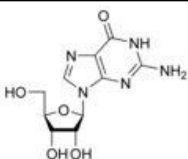
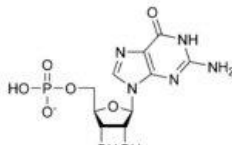
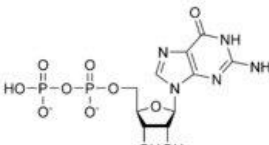
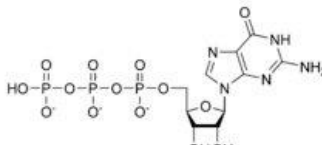
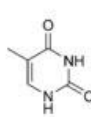
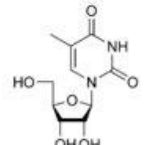
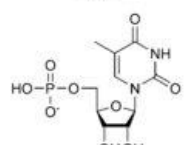
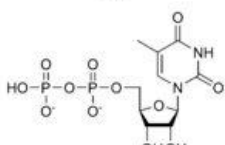
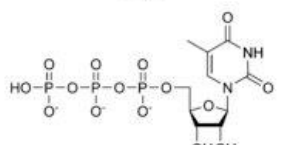
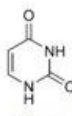
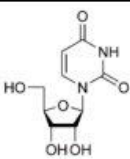
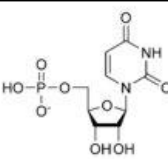
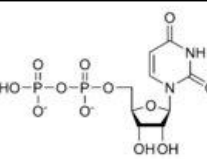
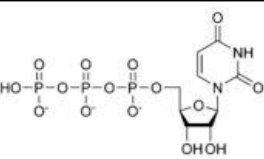
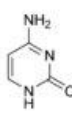
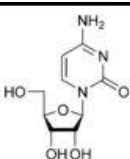
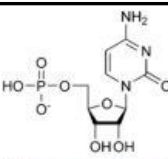
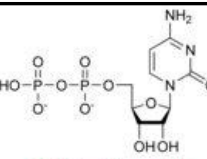
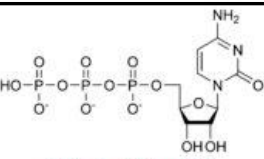


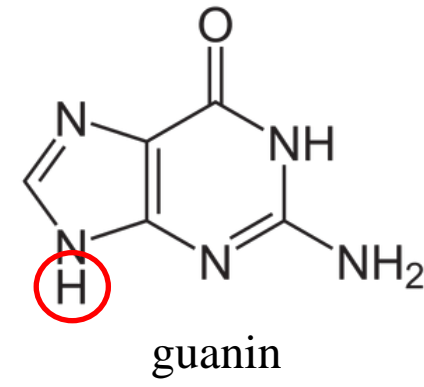
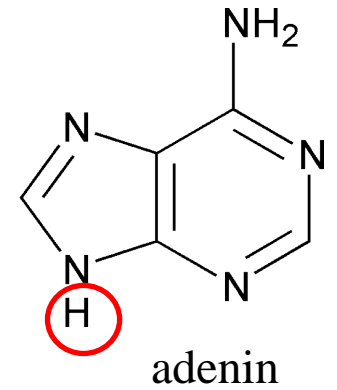
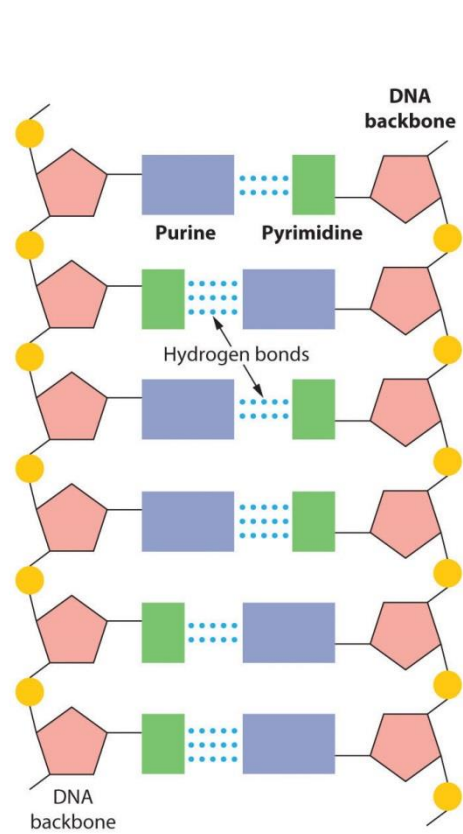
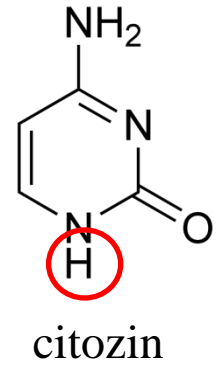
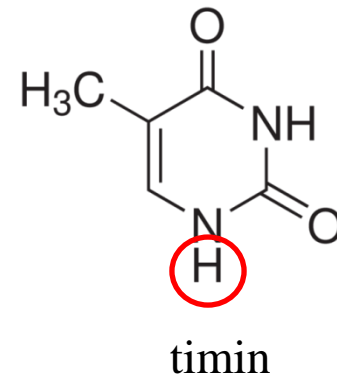
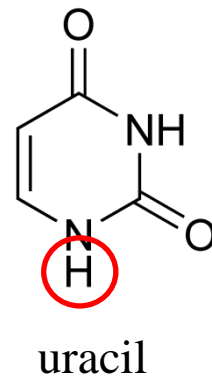
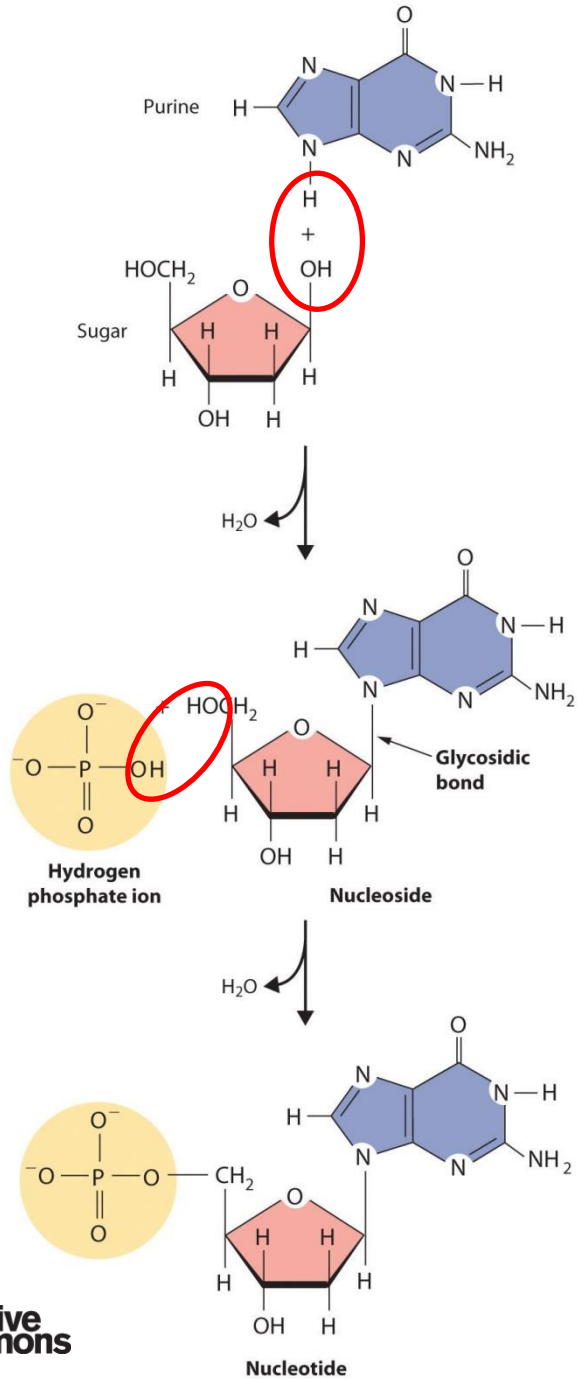
Q=OH
Q=H

adenozin-5'-monofoszfát
deziadenozin-5'-monofoszfát

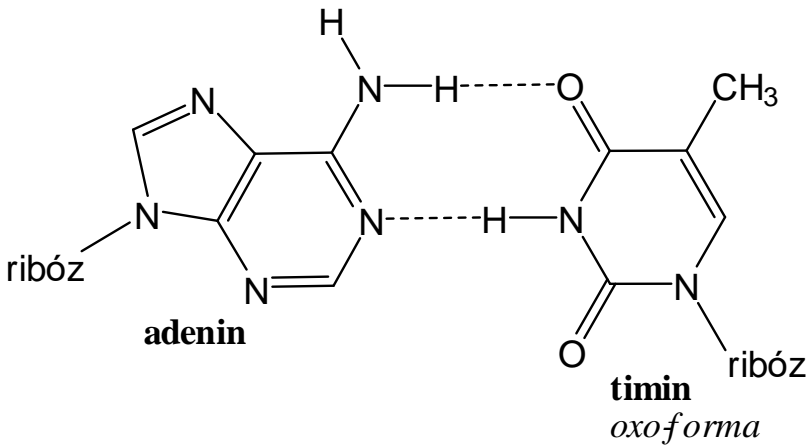
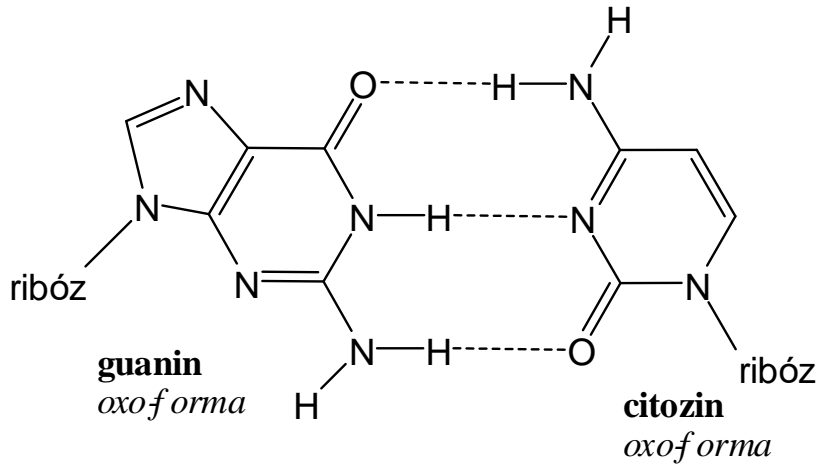
Nukleotidok:

A nukleozidok foszforsavészterei

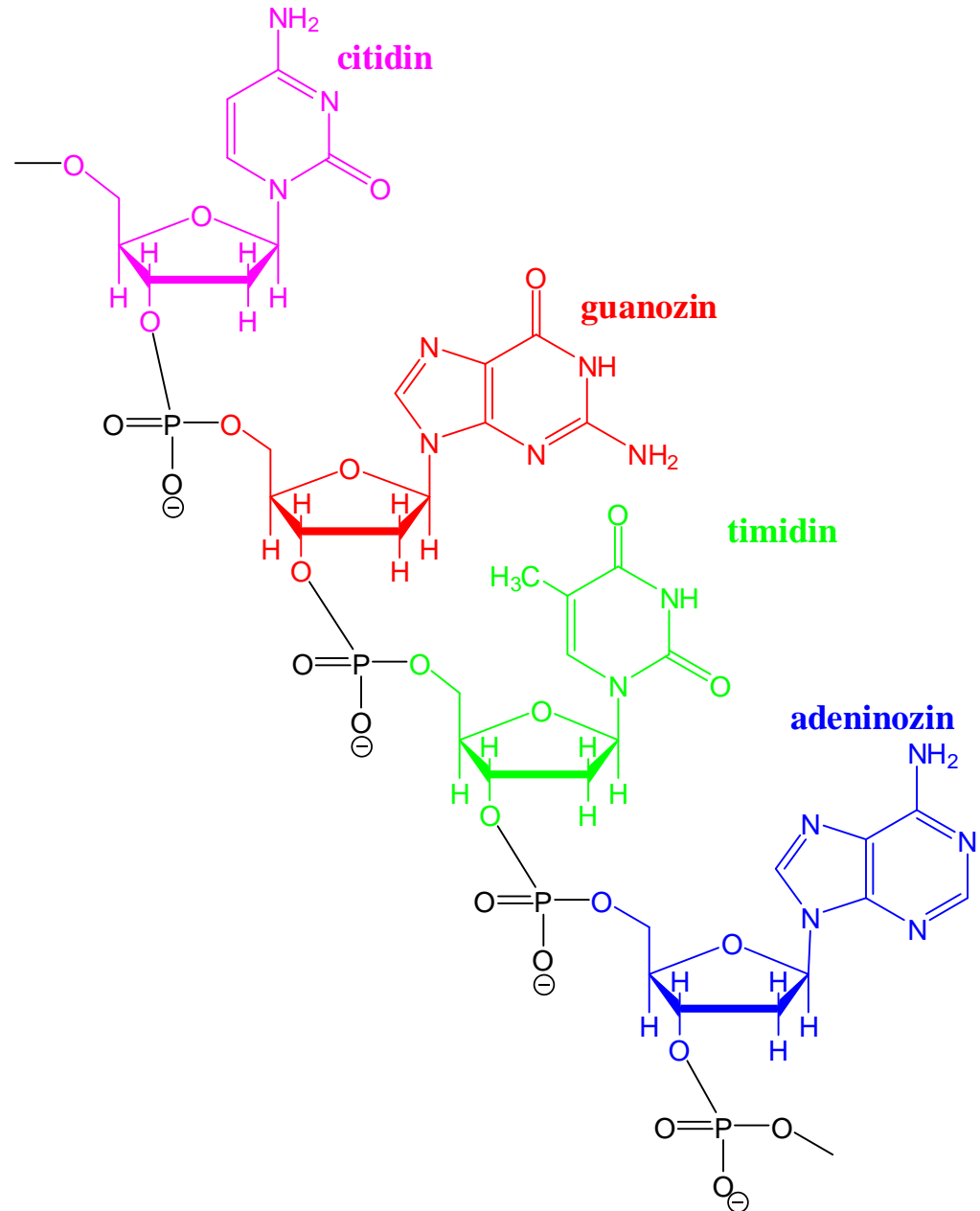
Nukleobázis	Nukleozid	5'- Nukleotidok		
 Adenin	 Adenozin A	 Adenozin-monofoszfát AMP	 Adenozin-difoszfát ADP	 Adenozin-trifoszfát ATP
 Guanin	 Guanozin G	 Guanozin-monofoszfát GMP	 Guanozin-difoszfát GDP	 Guanozin-trifoszfát GTP
 Timin	 Timidin T	 Timidin-monofoszfát TMP	 Timidin-difoszfát TDP	 Timidin-trifoszfát TTP
 Uracil	 Uridin U	 Uridin-monofoszfát UMP	 Uridin-difoszfát UDP	 Uridin-trifoszfát UTP
 Citozin	 Citidin C	 Citidin-monofoszfát CMP	 Citidin-difoszfát CDP	 Citidin-trifoszfát CTP



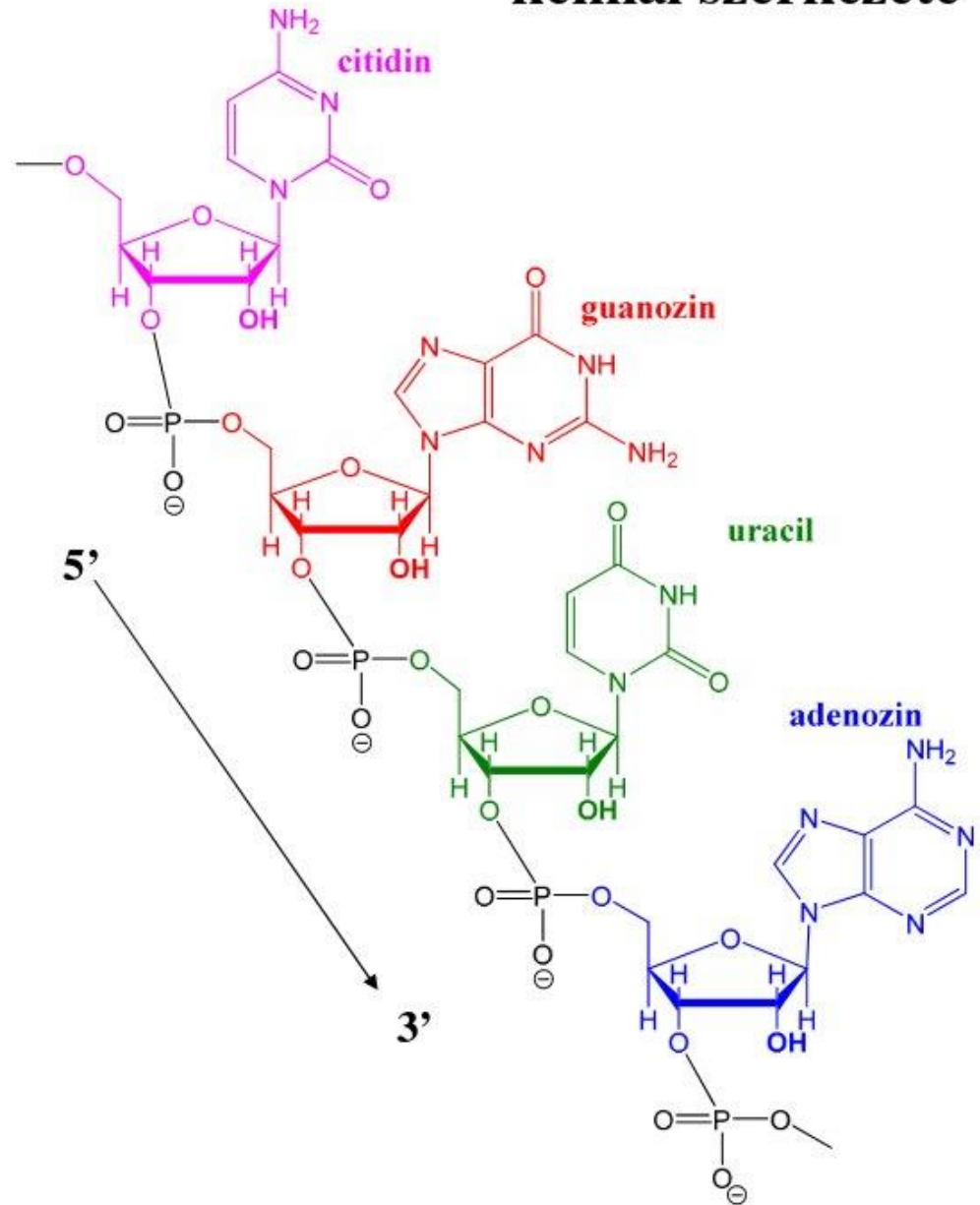
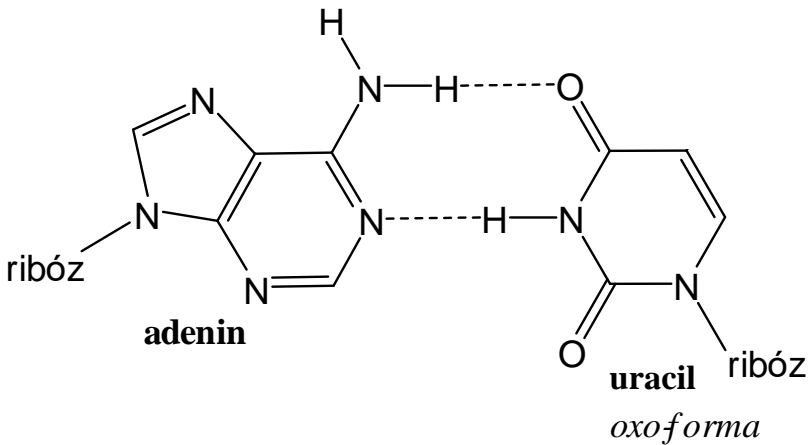
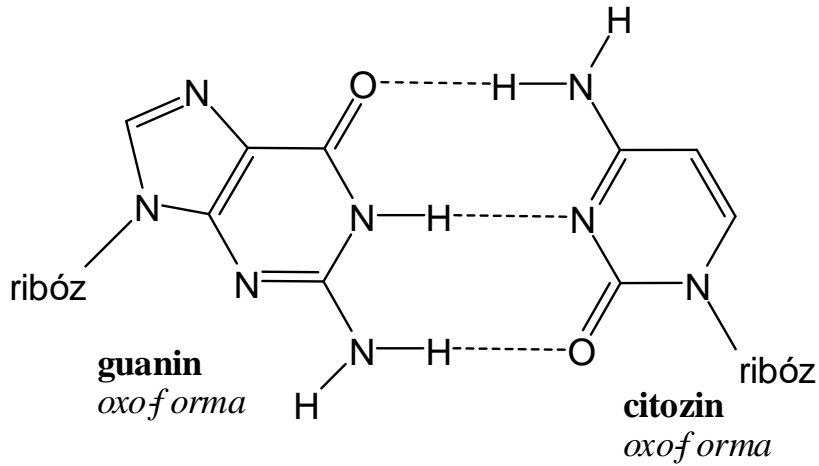
A Watson-Crick bázispárok: G-C és A-T



A DNS kémiai szerkezete:



Az RNS kémiai szerkezete



A DNS bázispárjai

timin

adenin

2,8 Å

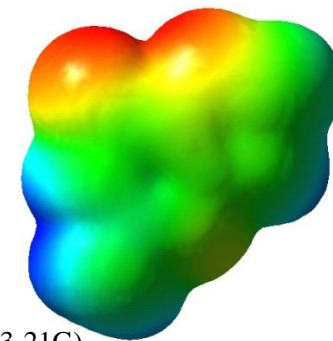
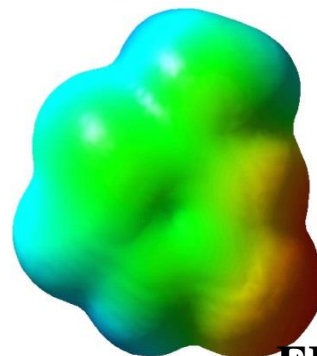
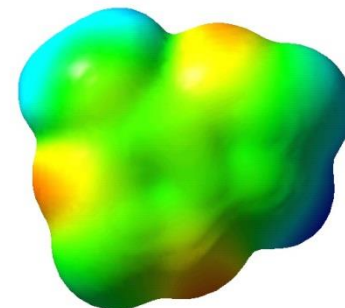
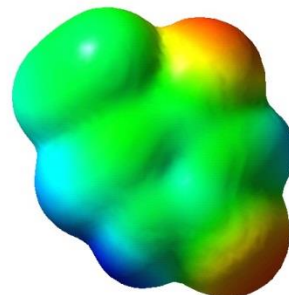
3,0 Å

citozin

guanin

2,8 Å

3,0 Å



EPS^(RHF/3-21G)

$-0.08 \pm 0.1 \leq \text{töltés} \leq 0.08 \pm 0.1$

2-dezoxi-β-D-ribófuranóz



HO

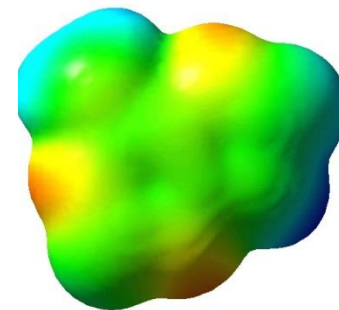
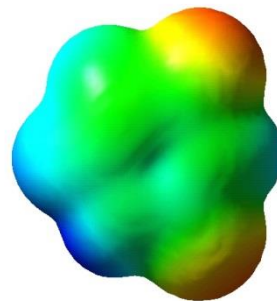
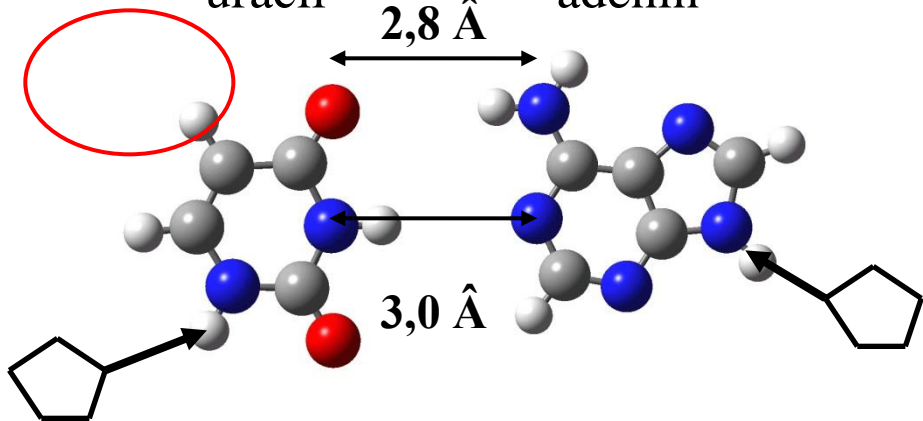
5-Hydroxymethyl-
tetrahydrofuran-2,4-diol

Az RNS bázispárjai

uracil adenin

2,8 Å

3,0 Å

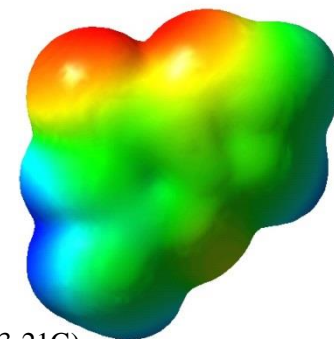
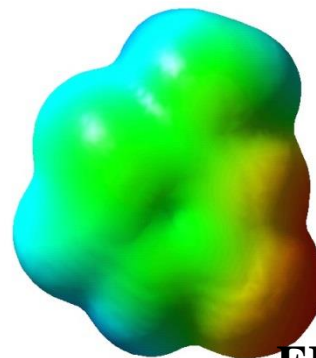
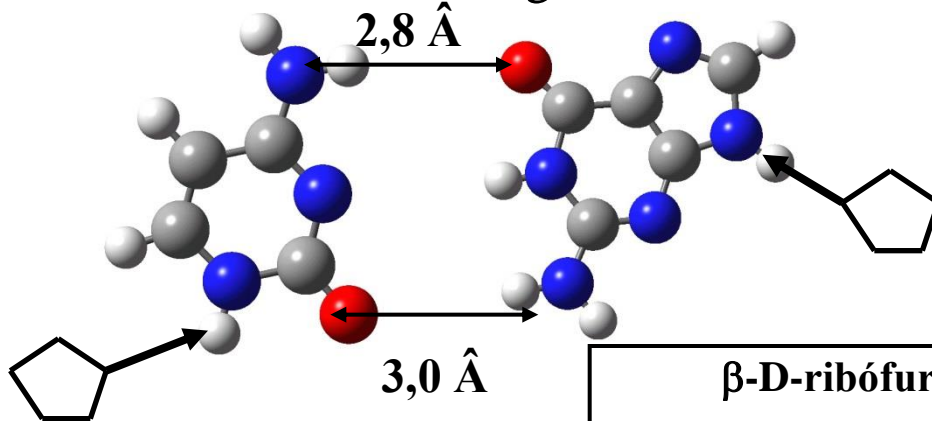


citozin

guanin

2,8 Å

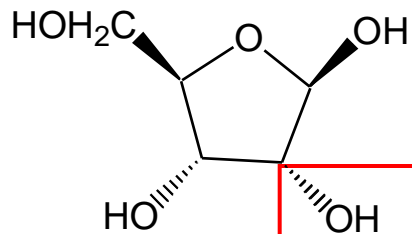
3,0 Å



EPS^(RHF/3-21G)

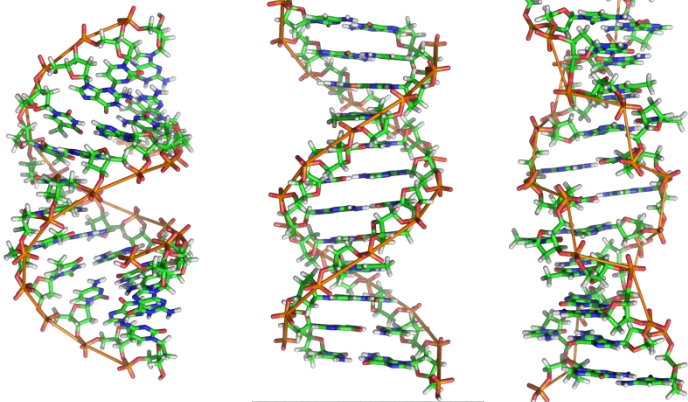
$-0.08 \pm 0.1 \leq \text{töltés} \leq 0.08 \pm 0.1$

β-D-ribófuranóz



5-Hydroxymethyl-
tetrahydrofuran-2,3,4-triol

A-, B-, Z-DNS



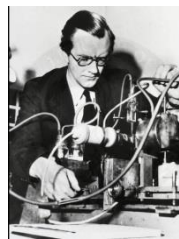
King's College



Rosalind Franklin

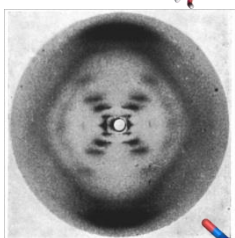
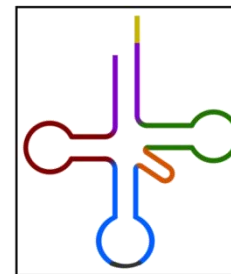
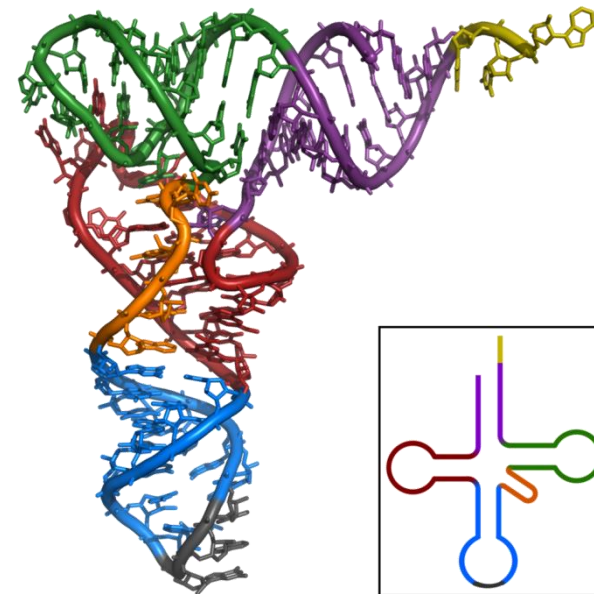


Raymond Gosling



Maurice Wilkins

tRNS



1952/1953
Nature

Cambridge



Francis és James
Crick Watson

2013 Nature Chemistry 5, 182.



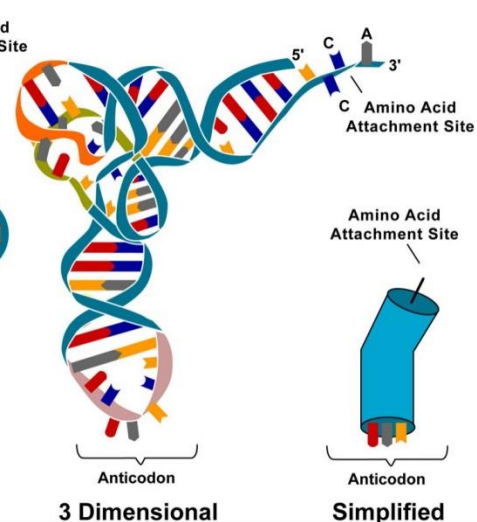
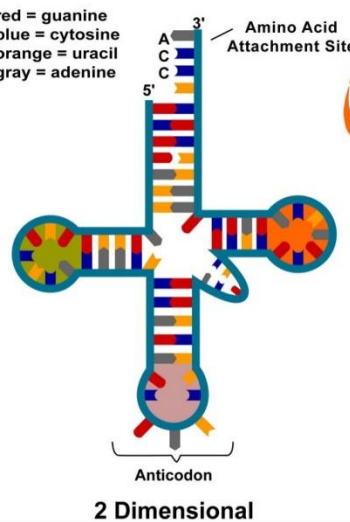
Shankar Balasubramanian

Cambridge

DNS-kvadruplex

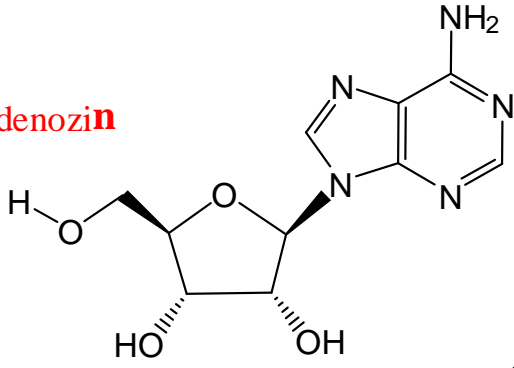
(guanin-gazdag telomér szekvenciákban:
proliferáció során különösen – rákterápia (?))

red = guanine
 blue = cytosine
 orange = uracil
 gray = adenine



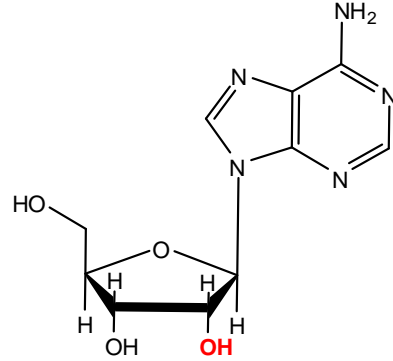
RNS építőelem

adenozin

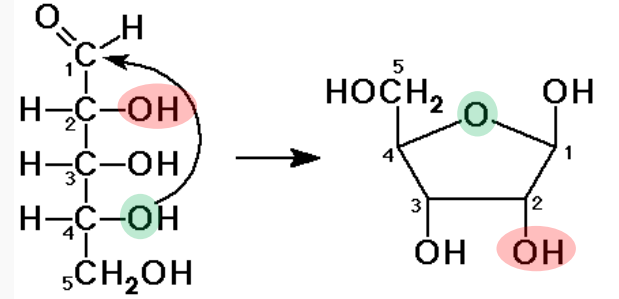


adenozin

9-(β-D-ribofuranozil)-adenin op= 235°C



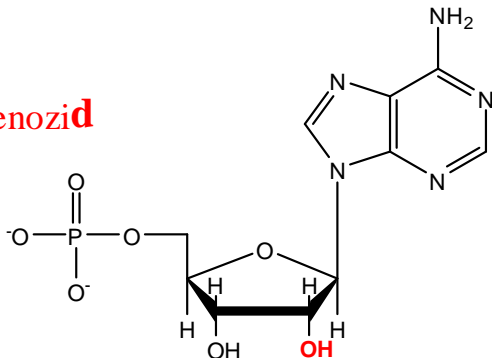
A cukoregység:



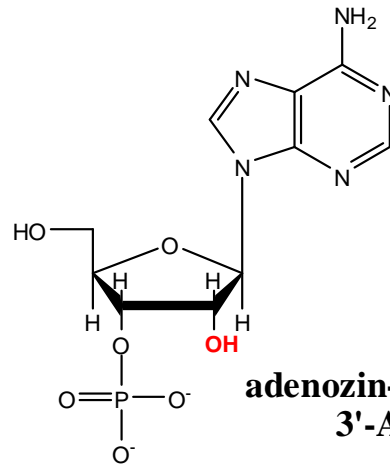
D-ribose

β-D-ribofuranose

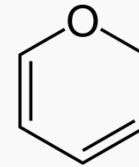
adenozid



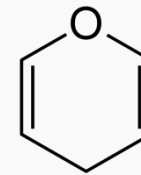
adenozin-5'-foszfát
5'-AMP



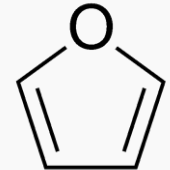
adenozin-3'-foszfát
3'-AMP



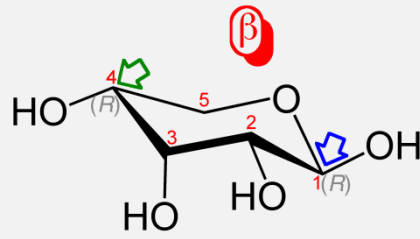
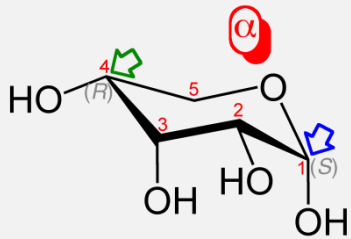
2H-pirán



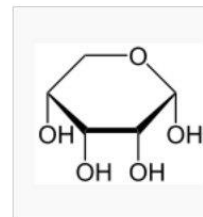
4H-pirán



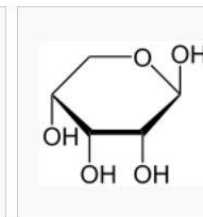
furán



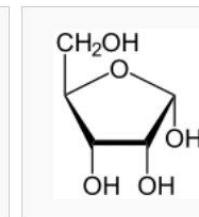
vízben: ~



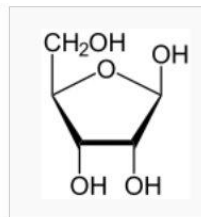
20%



60%

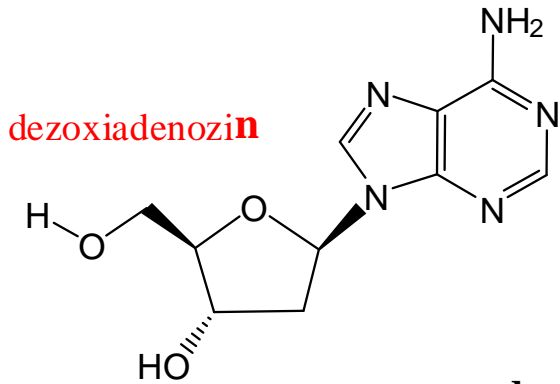


7%



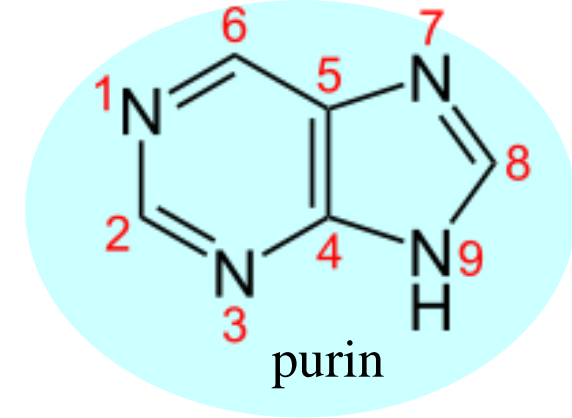
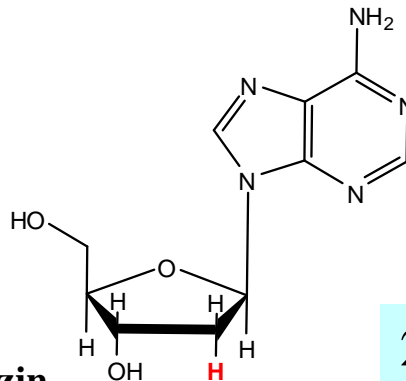
13%

DNS építőelem



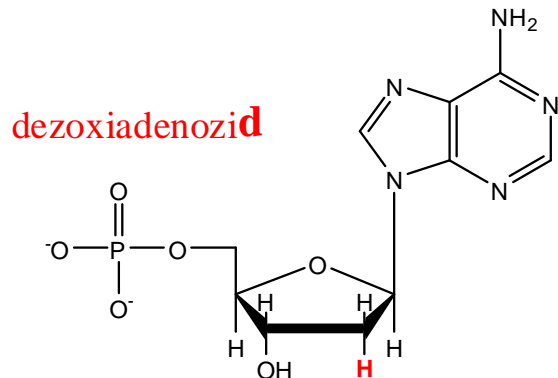
dezoxiadenozin

9-(2'-dezoxi-β-D-ribofuranozil)-adenin op= 190°C

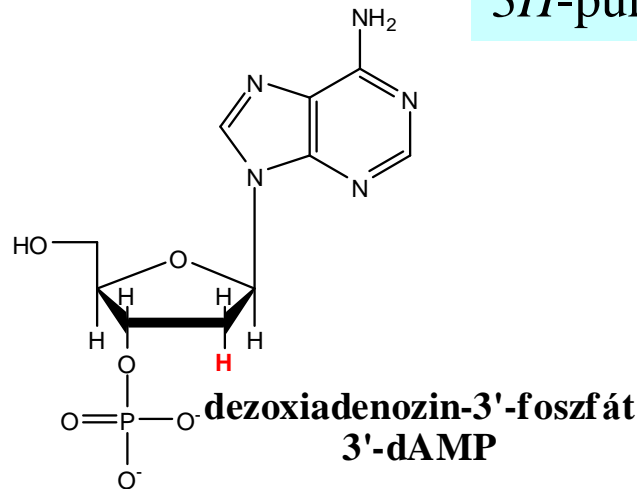


purin

2-Amino-9-[3,4-dihidroxi-5-(hidroximetil)tetrahidrofuran-2-il]-3*H*-purin-6-on



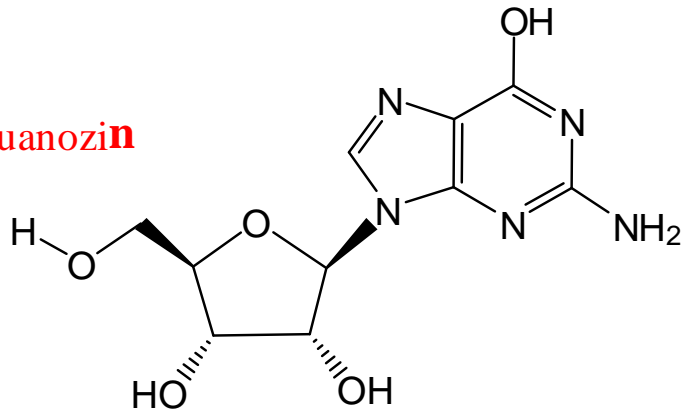
dezoxiadenozin-5'-foszfát
5'-dAMP



dezoxiadenozin-3'-foszfát
3'-dAMP

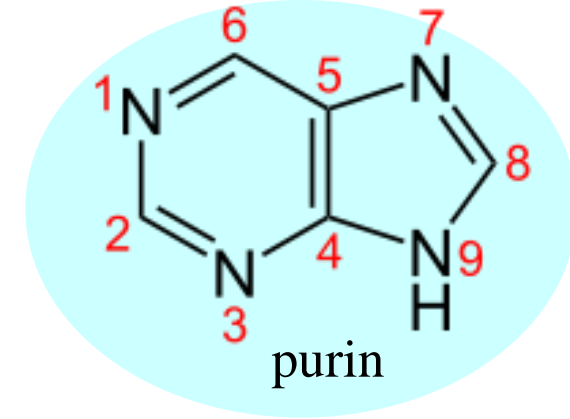
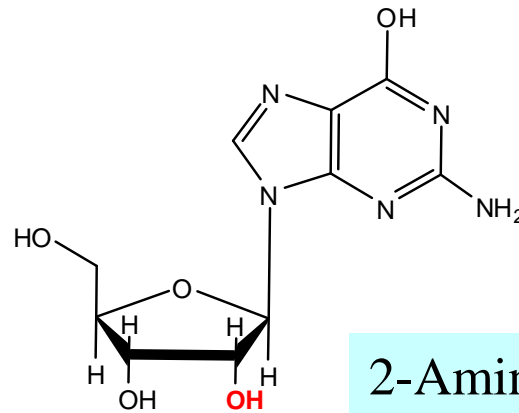
RNS építőelem

guanozin



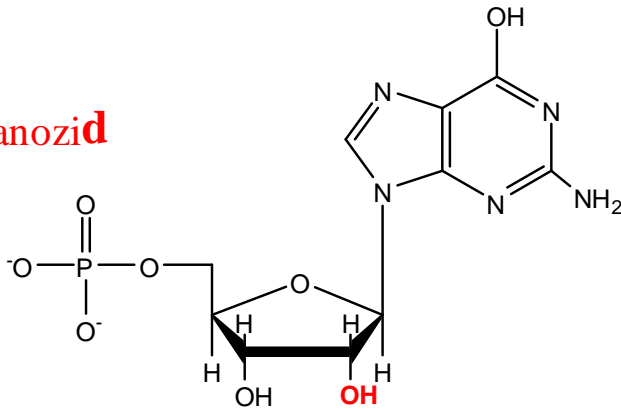
guanozin

9-(β-D-ribofuranozil)-guanin op= 240°C

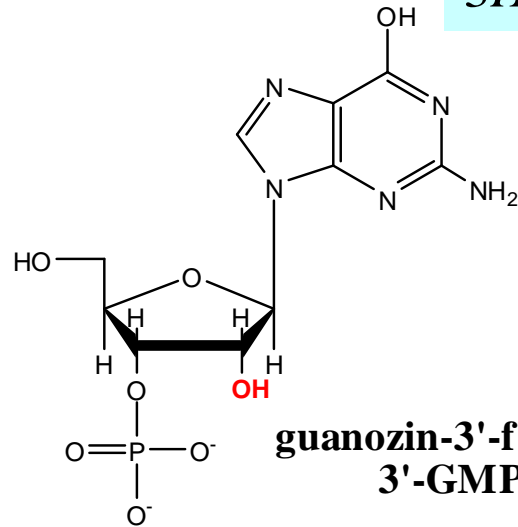


2-Amino-9-[3,4-dihidroxi-5-(hidroximetil)tetrahidrofuran-2-il]-3*H*-purin-6-on

guanozid

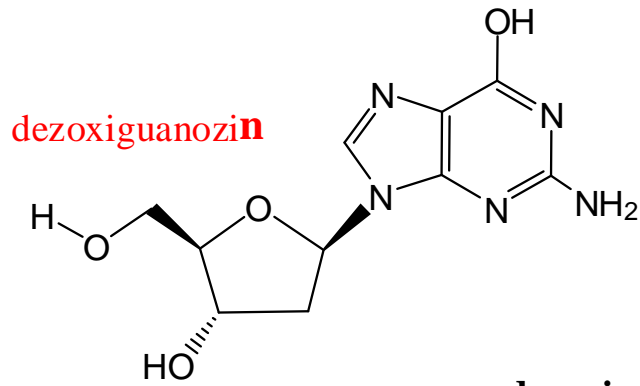
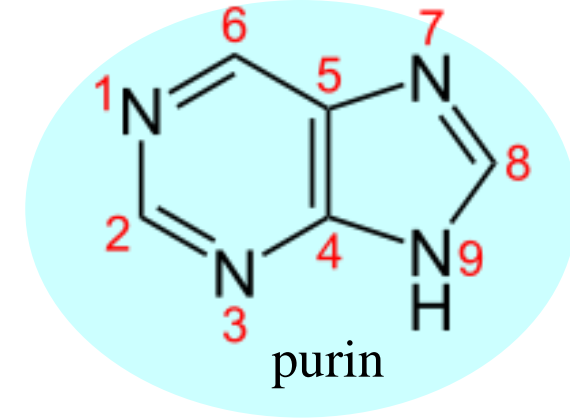


guanozin-5'-foszfát
5'-GMP

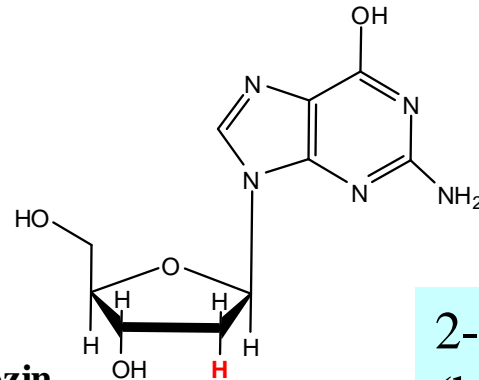


guanozin-3'-foszfát
3'-GMP

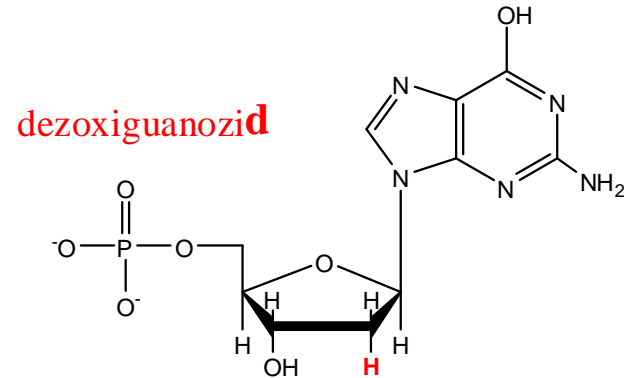
DNS építőelem



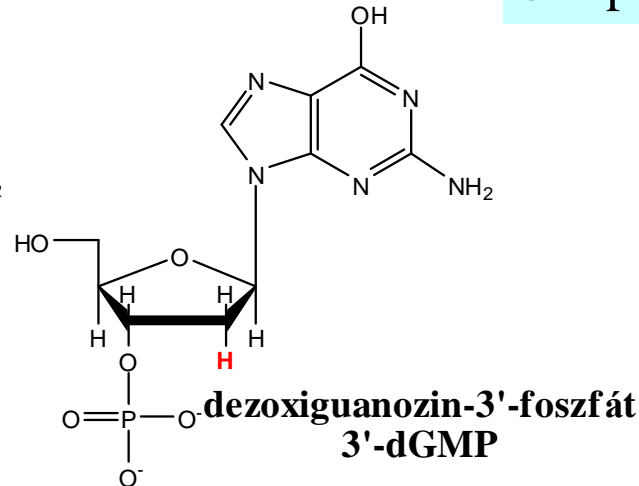
deoxiguanozin
9-(2'-dezoxi-β-D-ribofuranozil)-guanin



2-Amino-9-[4-hidroxi-5-(hidroximetil)tetrahidrofuran-2-il]-3*H*-purin-6-on

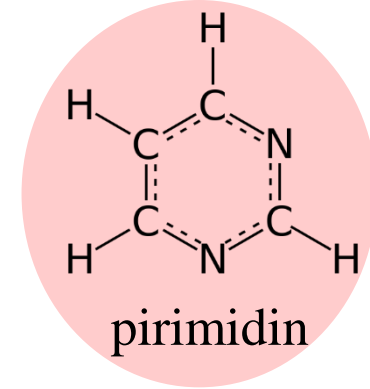
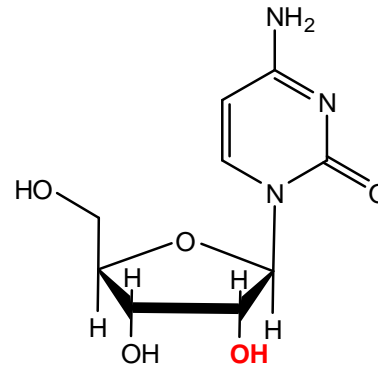
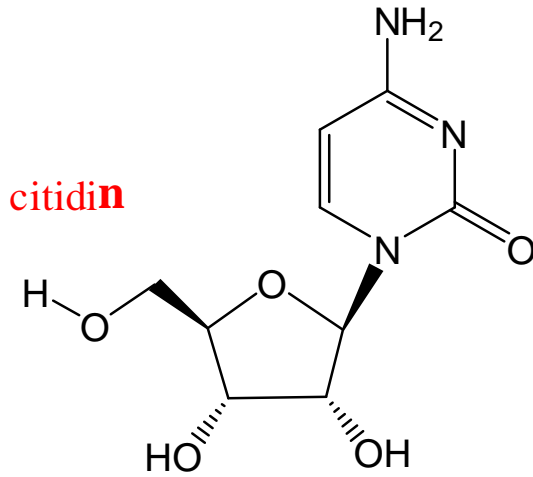


deoxiguanozin-5'-foszfát
5'-dGMP



deoxiguanozin-3'-foszfát
3'-dGMP

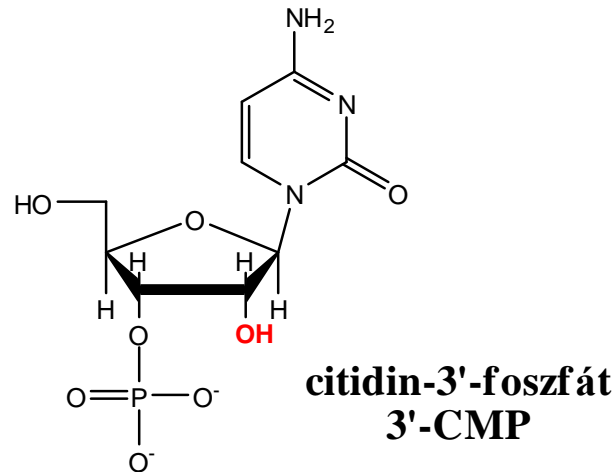
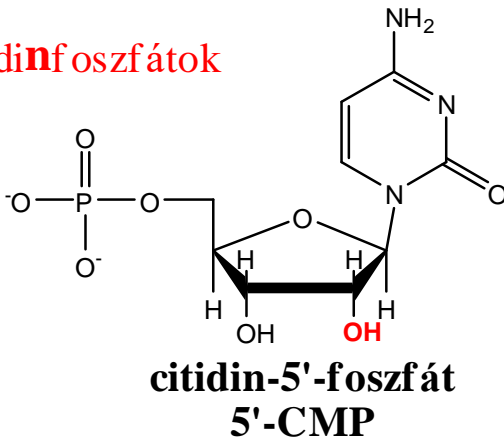
RNS építőelem



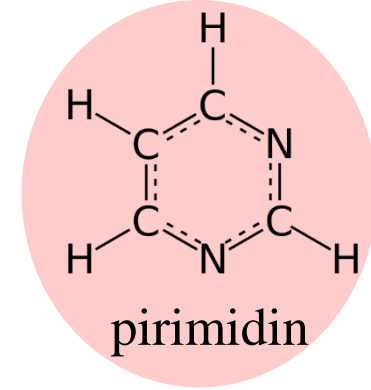
3-(β -D-ribofuranozil)-citozin op= 230°C

4-amino-1-[3,4-dihidroxi-5-(hidroximetil)tetrahidrofuran-2-il]pirimidin-2-on

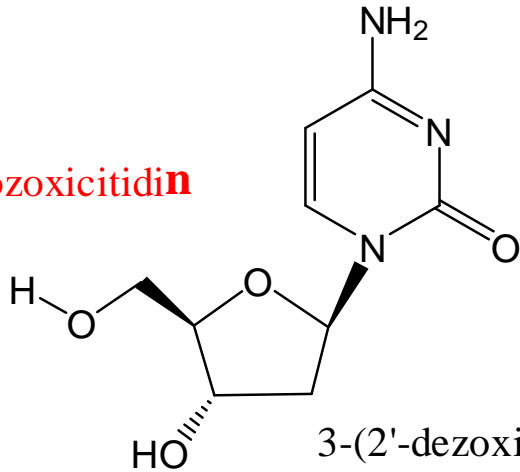
citidin foszfátok



DNS építőelem

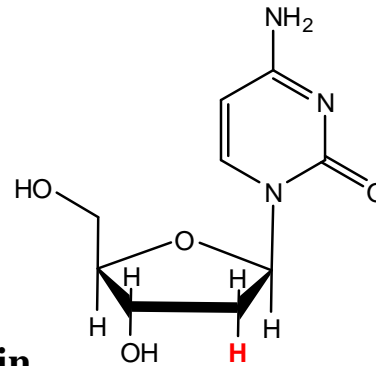


dozoxicitidin



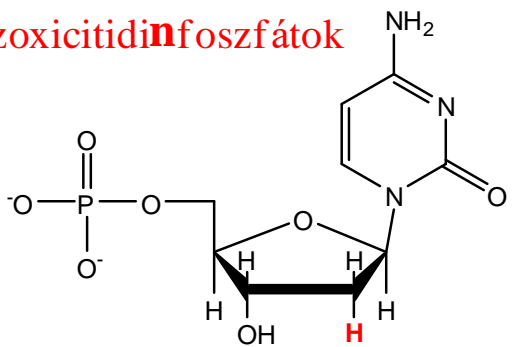
dezoxicitidin

3-(2'-deoxi-β-D-ribofuranozil)-citozin

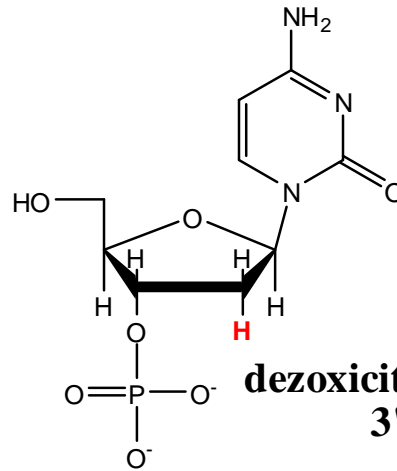


4-amino-1-[3-hidroxi-5-(hidroximetil)tetrahidrofuran-2-il]pirimidin-2-on

dezoxicitidinfoszfátok



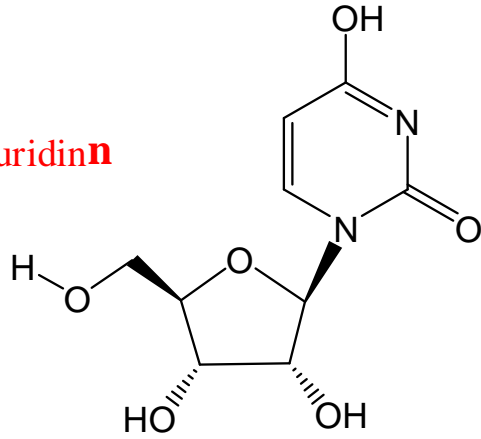
dezoxicitidin-5'-foszfát
5'-dCMP



dezoxicitidin-3'-foszfát
3'-dCMP

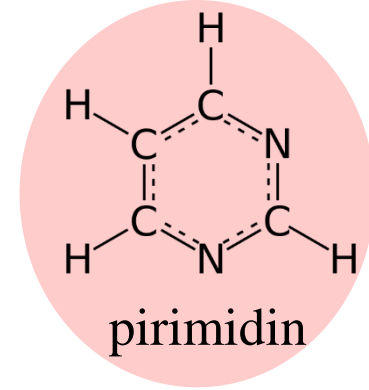
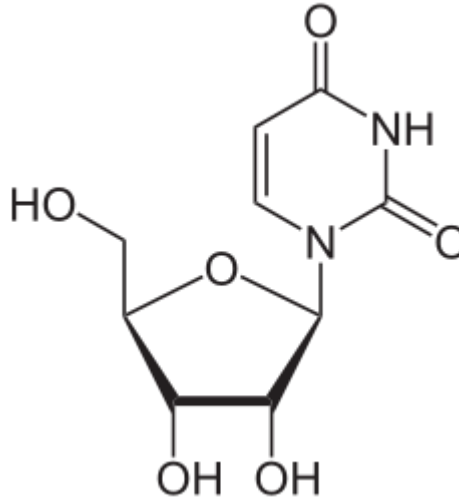
RNS építőelem

uridin



uridin

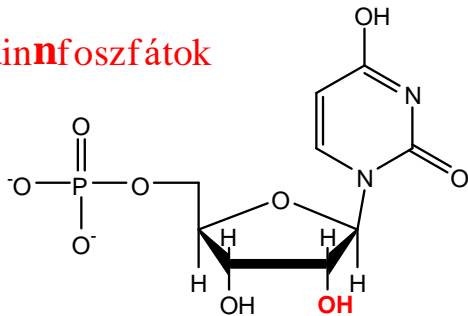
3-(β-D-ribofuranosil)-uracil op= 165°C



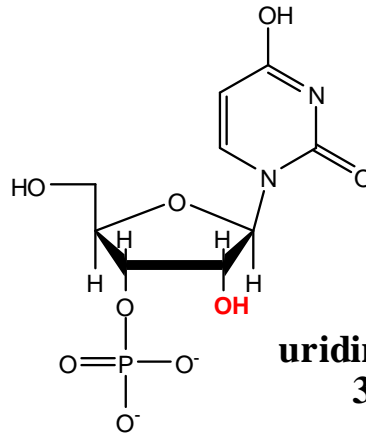
pirimidin

1-[3,4-dihidroxi-5-(hidroximetil)tetrahidrofuran-2-il]pirimidin-2,4-dion

uridin foszfátok

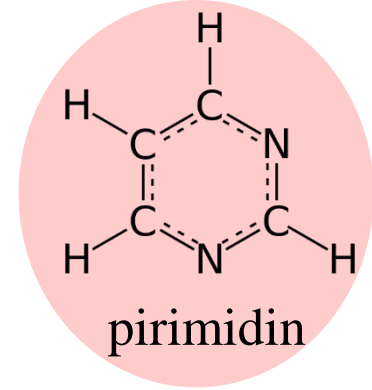


uridin-5'-foszfát
5'-UMP

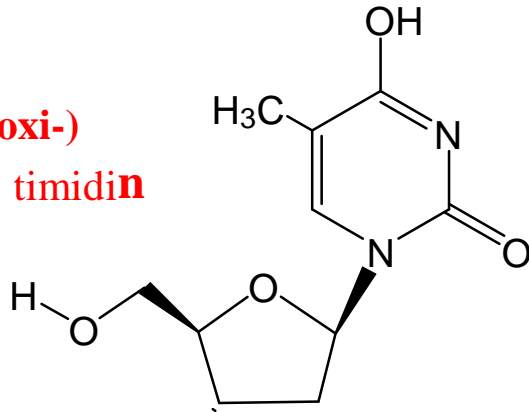


uridin-3'-foszfát
3'-UMP

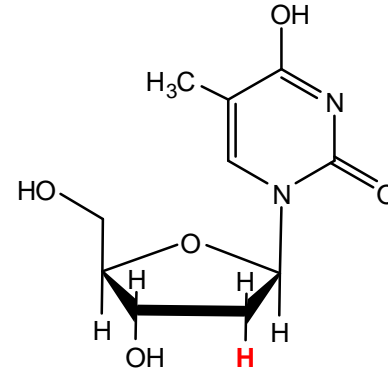
DNS építőelem



(dezoxi-)
timidin



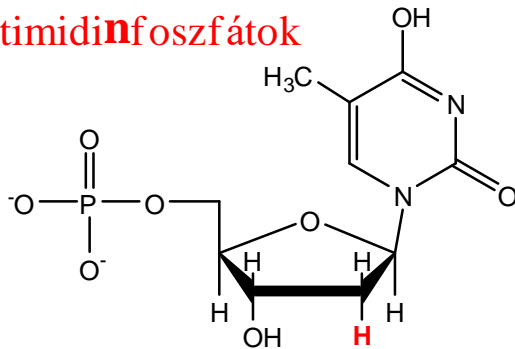
timidin



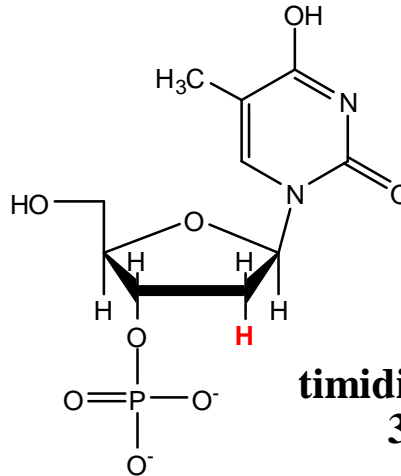
HO 3-(2'-dezoxi-β-D-ribofuranozil)-timin op= 183°

5-metil-1-[4-hidroxi-5-(hidroximetil)tetrahidrofuran-2-il]-pirimidin-2,4-dion

timidinofoszfátok

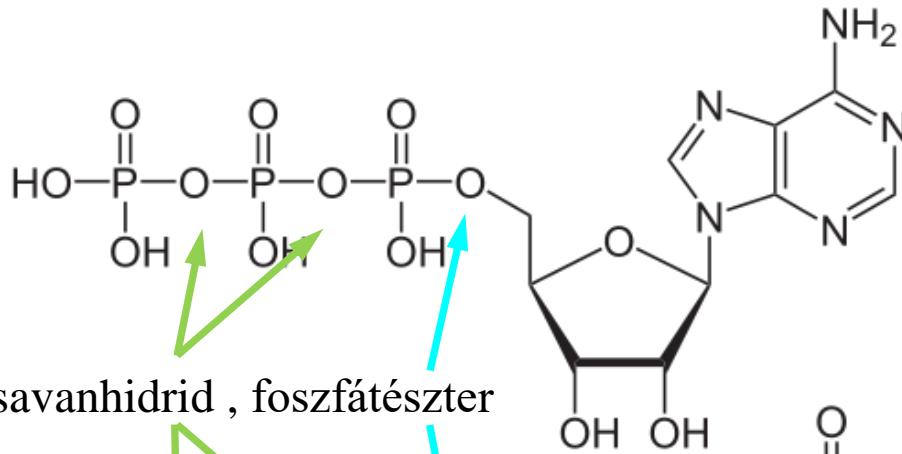


timidin-5'-foszfát
5'-TMP



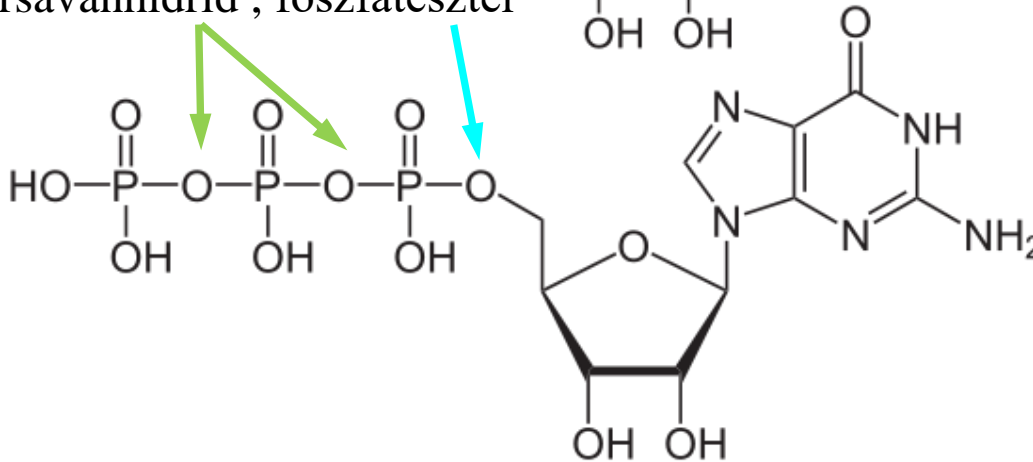
timidin-3'-foszfát
3'-TMP

A szervezet energiatárolói („elemei”): ATP, GTP

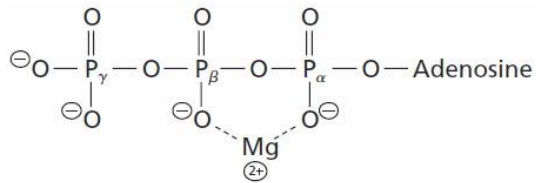


ATP: adenzin-5'-trifoszfát

foszforsavanhidrid , foszfátészter

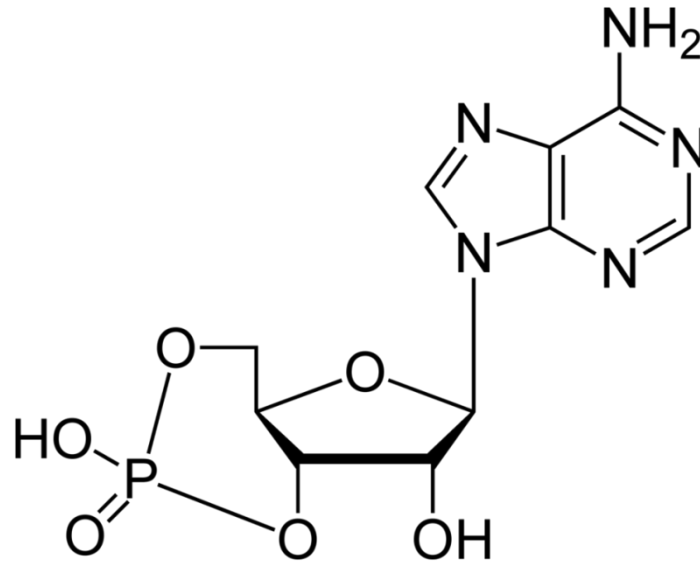


GTP: guanozin-5'-trifoszfát



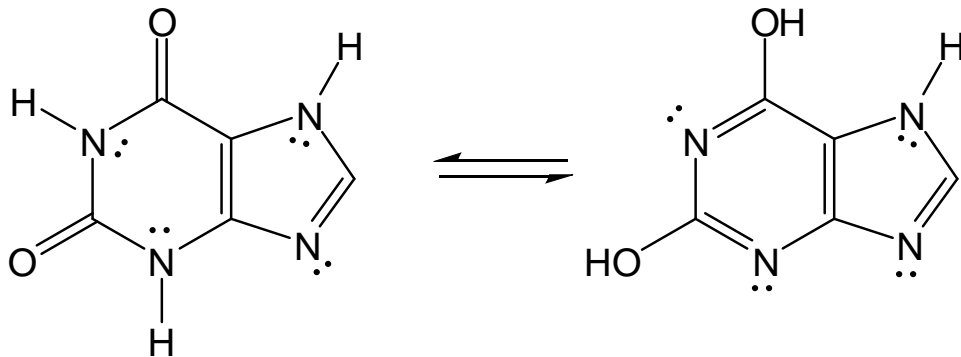
ATP \rightarrow ADP + P_i átalakulást kísérő szabadenergia változás:
~ -50 kJ/mol

Egy másodlagos hírvivő: cAMP



- jelátviteli folyamatokban vesz részt: glükagon, adrenalin hatását közvetíti a sejteken belülrre
- cukorháztartás, lipid-lebontás szabályzása

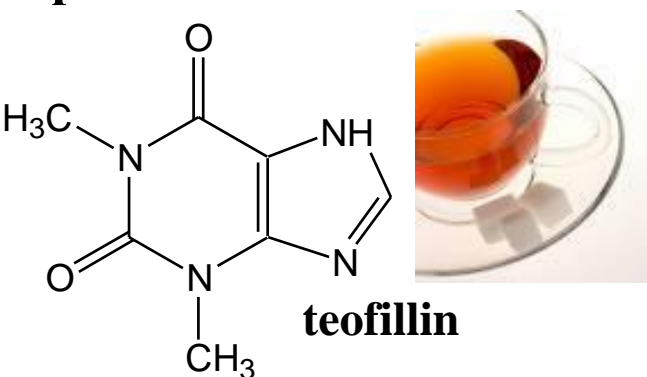
A **xantin** (purin-2,6-diol) két tautomer formája:



dilaktám forma
stabilabb

dilaktim forma
kevésbé stabil

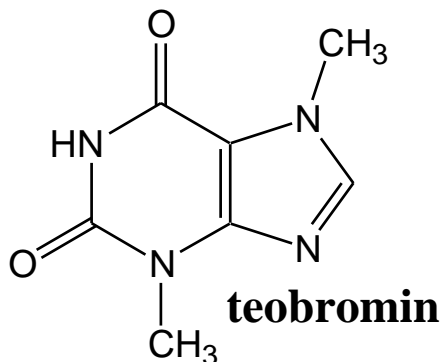
purinvázis alkaloidok: dimetil származékok



teofilin

1,3-dimetilxantin

1,3-Dimethyl-3,4,5,7-tetrahydro-
purine-2,6-dione



teobromin

3,7-dimetilxantin

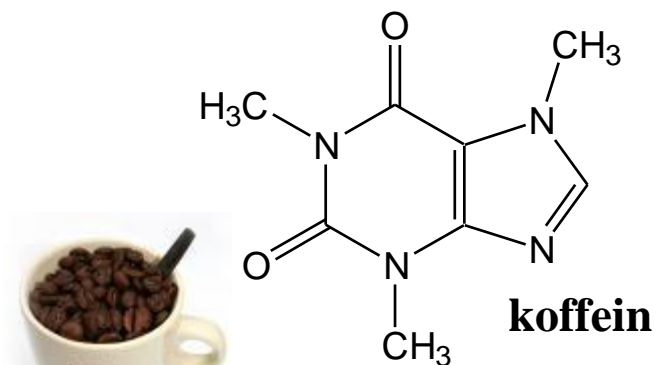
3,7-Dimethyl-3,4,5,7-tetrahydro-
purine-2,6-dione



- **koffein**: központi idegrendszer, szív – pszicho-stimulációs hatás
- **teofilin**: szív, simaizom – értágító, vízhajtó hatás
- **teobromin**: víhajtó, értágító, lazító hatás

foszfodiészteráz enzim inhibitora,
adenozin receptorok antagonistája
(cAMP, adrenalin, dopamin
szintnövekedés)

purinvázis alkaloidok:
a xantin **trimetil** származéka



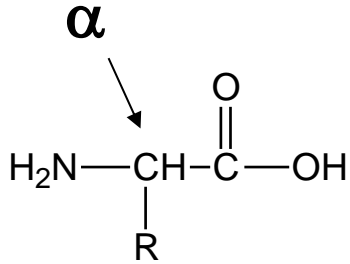
koffein

1,3,7-trimetilxantin

1,3,7-Trimethyl-3,4,5,7-tetrahydro-
purine-2,6-dione

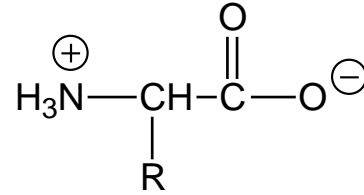
A) természetes aminosavak

Konstitúciója: α



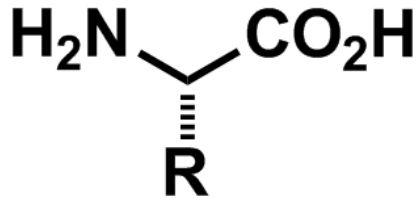
2-aminoalkánsav

ikerionos forma

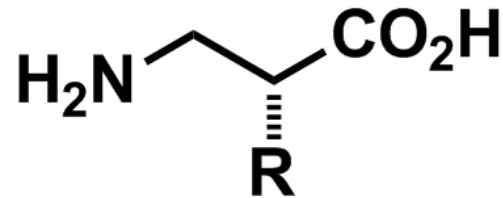


lehetne még...

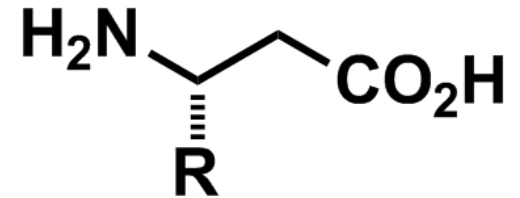
α -amino acid



β^2 -amino acid

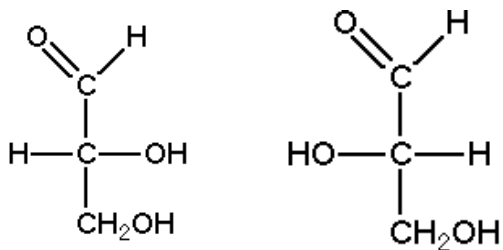


β^3 -amino acid

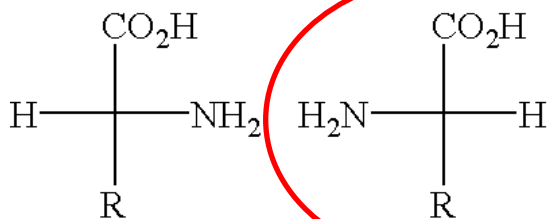


van is néha...

Konfigurációja: L

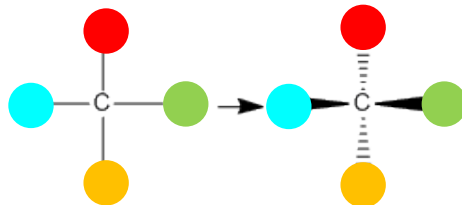


D-(+)-glicerinaldehid L-(-)-glicerinaldehid

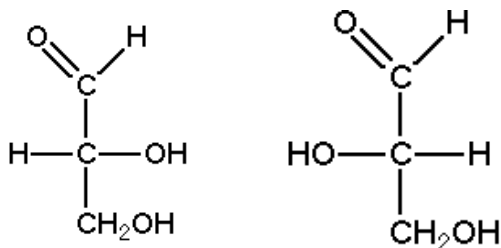


D-aminosavak L-aminosavak

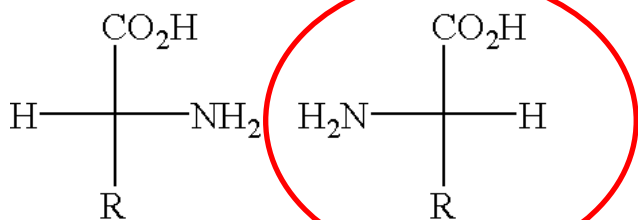
Fisher projekció



Konfigurációja: *L*

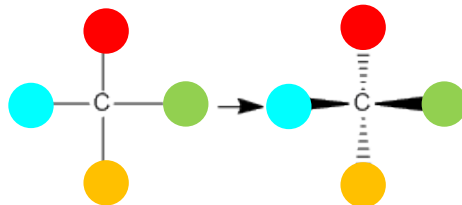


D-(+)-glicerinaldehid L-(-)-glicerinaldehid

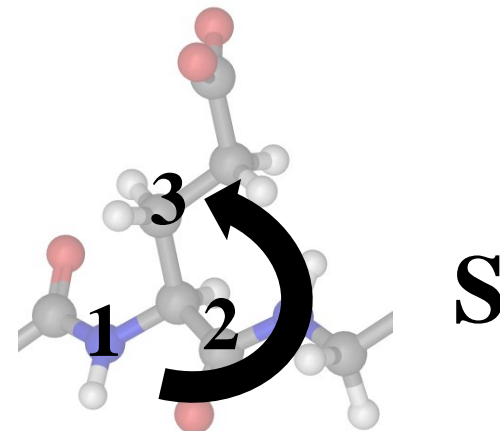


D-aminosavak L-aminosavak

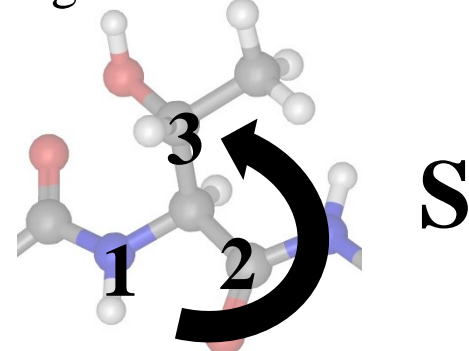
Fisher projekció



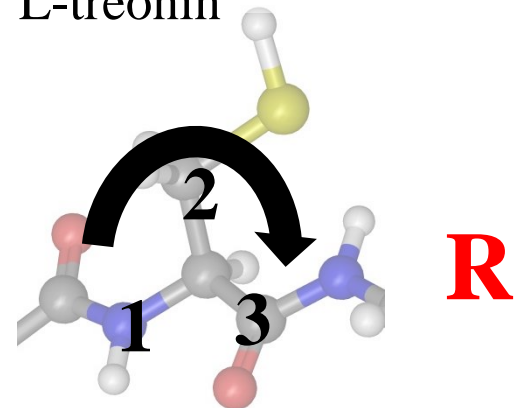
...azért van D-aminosav is: D-Ser, D-Asp, sőt: D-DOPA – skizofrénia patofiziológiája



L-glutaminsav



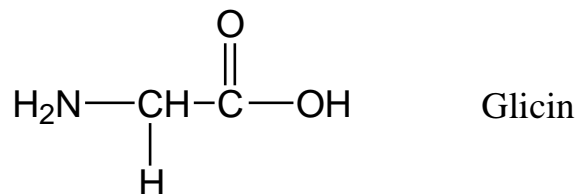
L-treonin



L-cisztein **kivétel !!!!!**

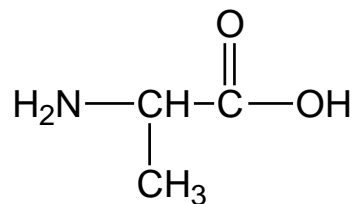
A legfontosabb természetes aminosavak

akirális

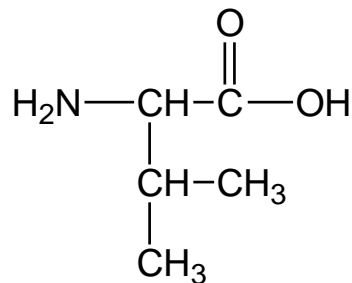


királis

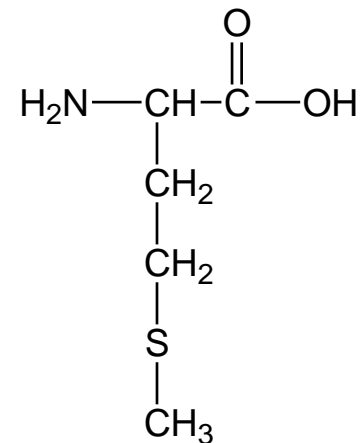
Alifás oldallácú hidrofób



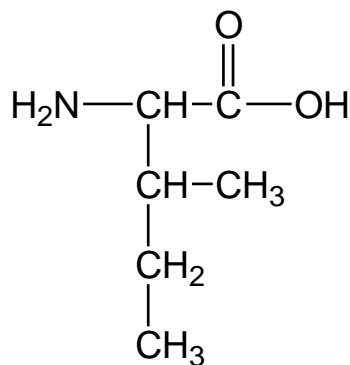
Alanin



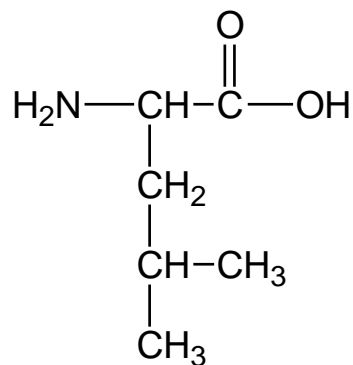
Valin



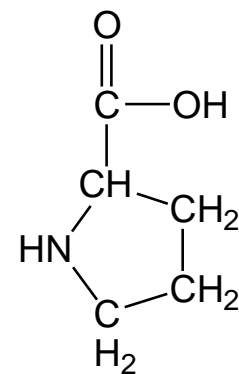
Metionin



Izoleucin

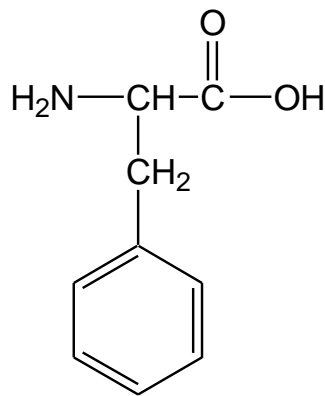


Leucin

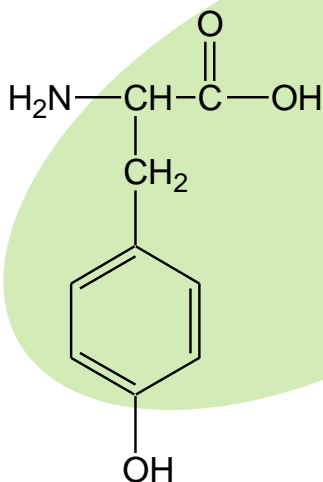


Prolin

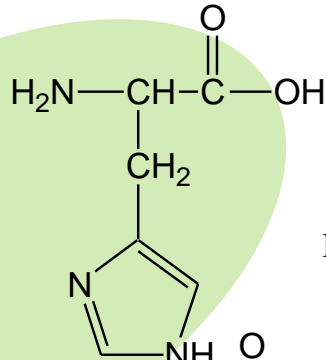
Aromás oldallácu hidrofób



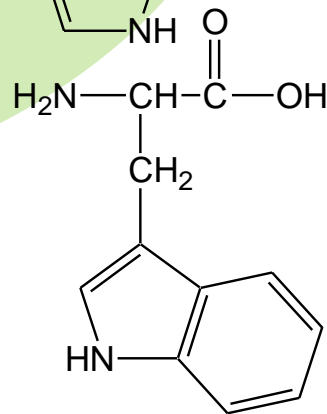
Fenilalanin



Tirozin

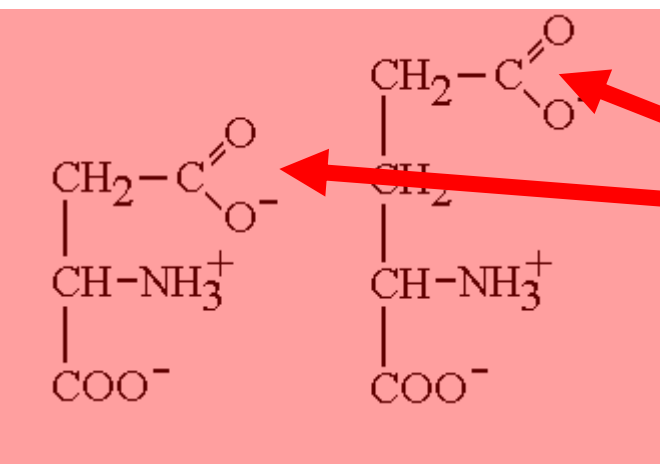


Hisztidin



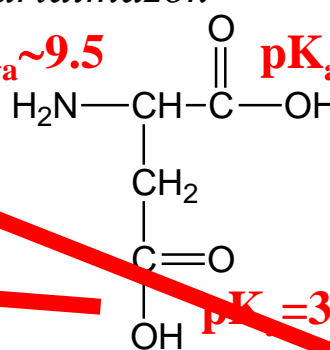
Triptofán

oldalláncban karbonil csoportot tartalmazók



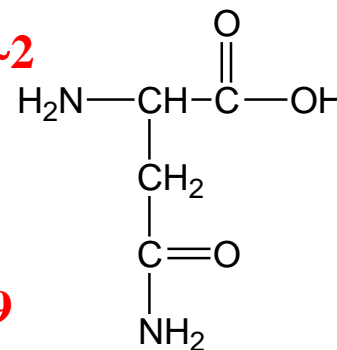
$pK_a \sim 9.5$

$pK_a \sim 2$

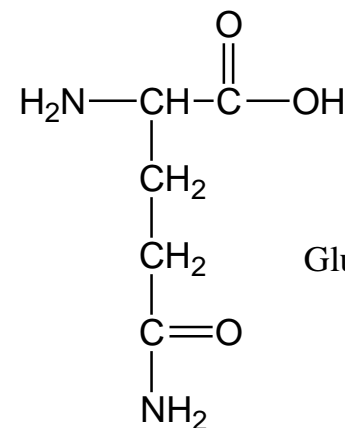


Aszparaginsav

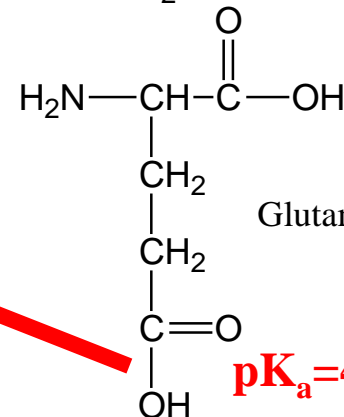
$pK_a = 3.9$



Aszparagin



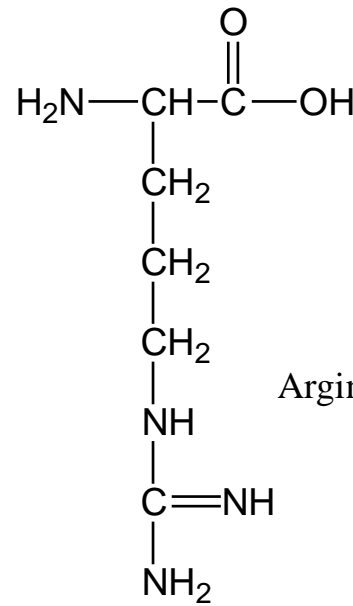
Glutamin



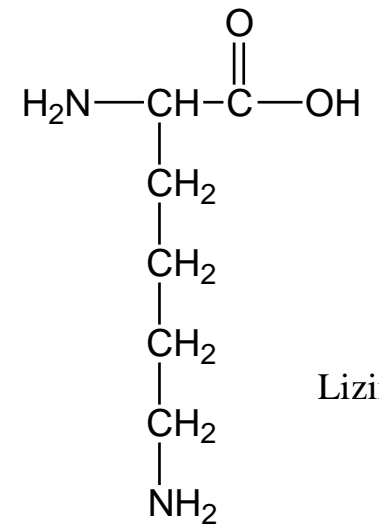
Glutaminsav

$pK_a = 4.1$

oldalláncban bázisos csoportot tartalmazók

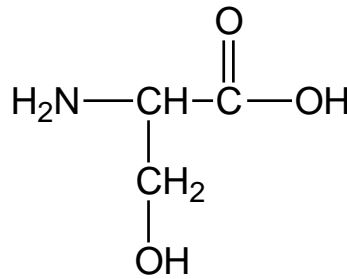


Arginin

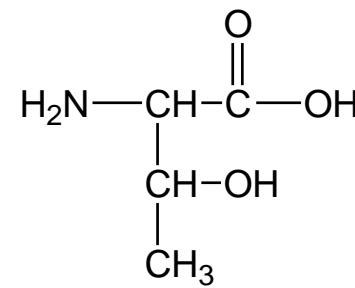


Lizin

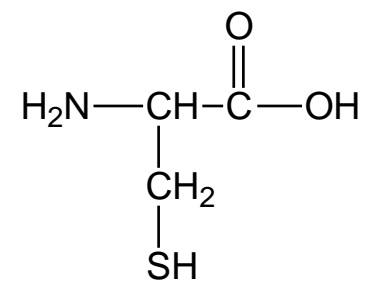
rövid poláris oldallánú csoportot tartalmazók



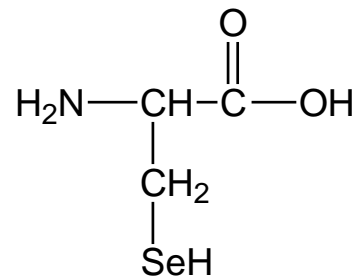
Szerin



Treonin

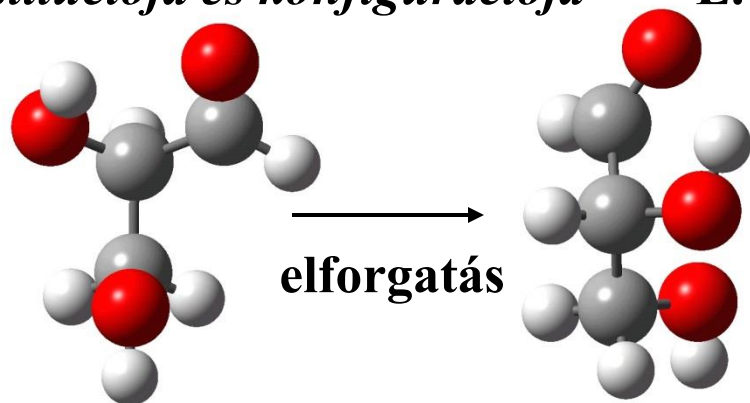


Cisztein



Szelenocisztein

Konstitúciója és konfigurációja

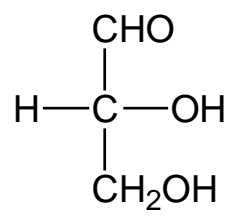


R

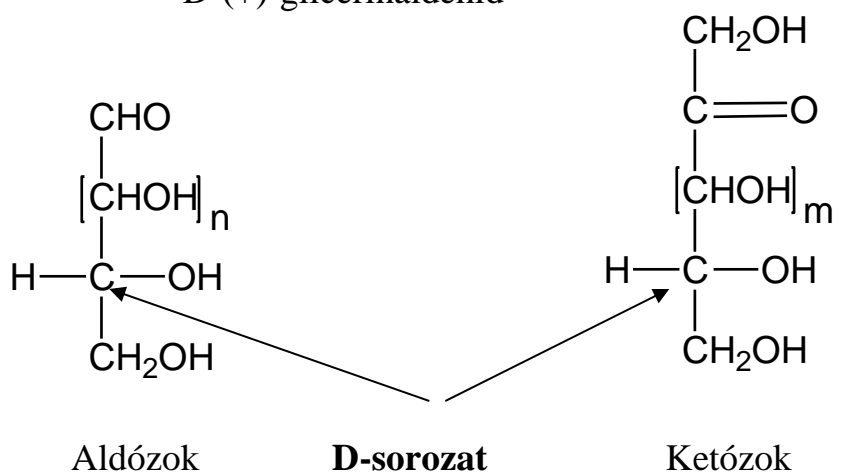
R

abszolút konfiguráció

E. Fischer féle projekció



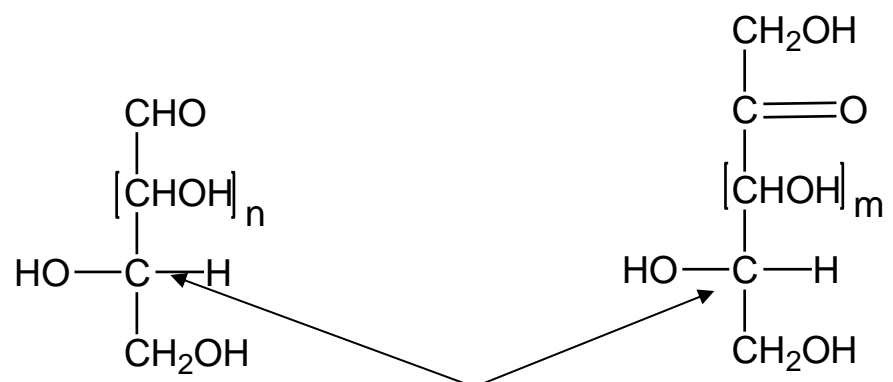
D-(+)-gliceraldehid



Aldózosok

D-sorozat

Ketózosok



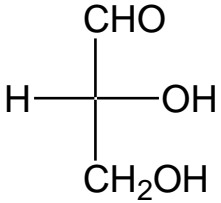
Aldózosok

L-sorozat

Ketózosok

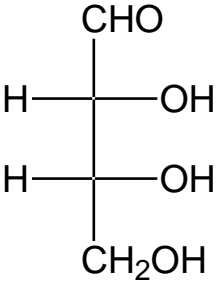
A legfontosabb cukrok nyílt formája

aldotrióz

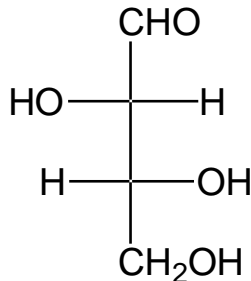


D-glicerinaldehid

aldotetróz

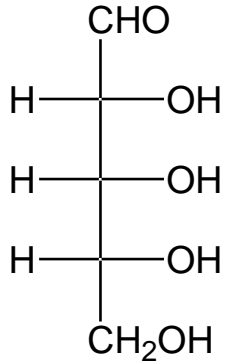


D-eritróz

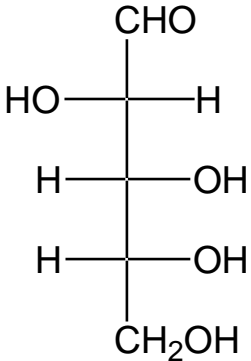


D-treóz

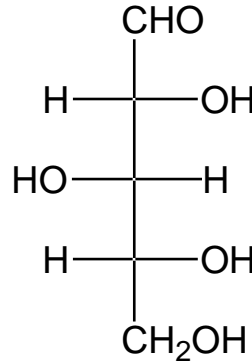
aldopentóz



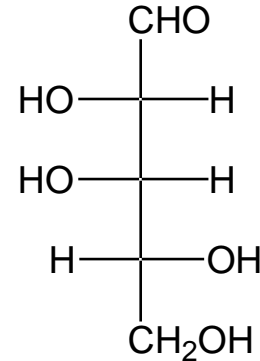
D-ribóz



D-arabinóz

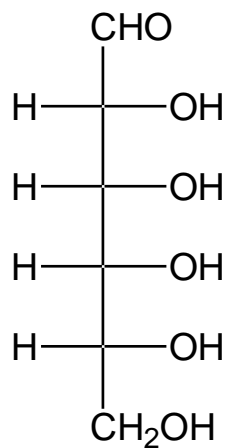


D-xilóz

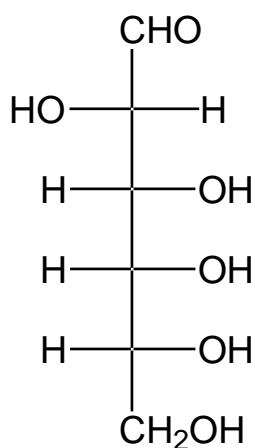


D-lixóz

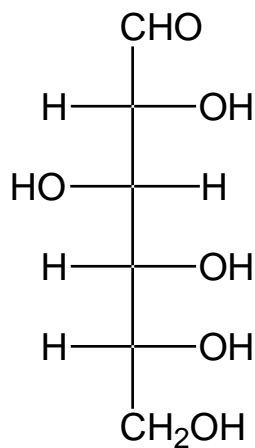
aldohexóz



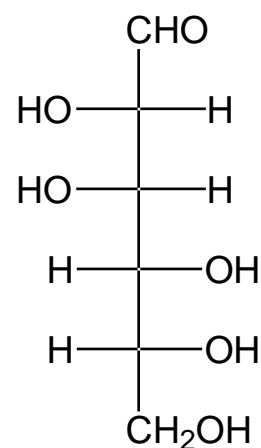
D-allóz



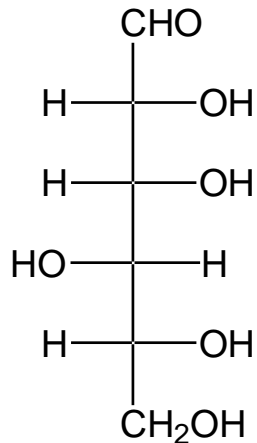
D-altróz



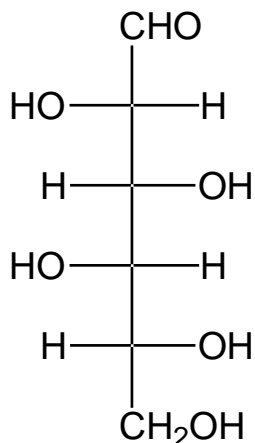
D-glükóz



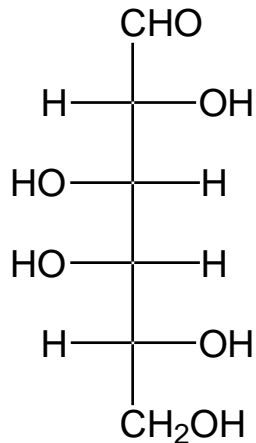
D-mannóz



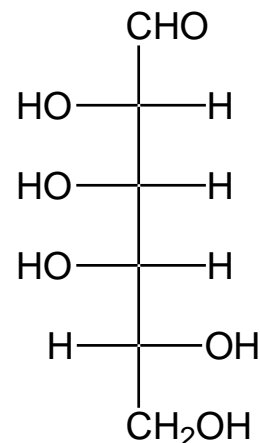
D-gulóz



D-idóz



D-galaktóz



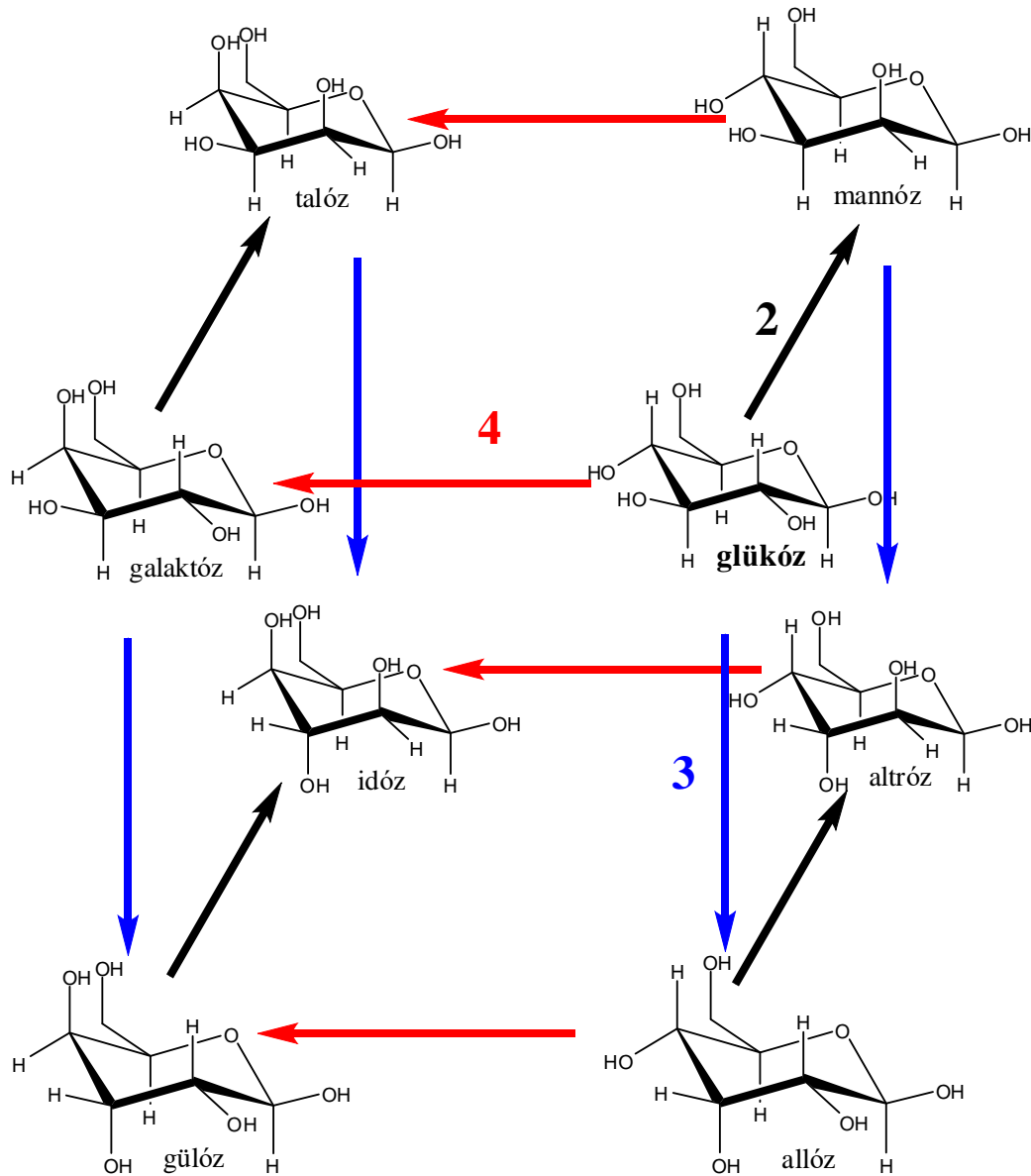
D-talóz

Nev.tan.: D-(+)-glükóz az

(+)-2R,3S,4R,5R-2,3,4,5,6-pentahidroxihexanal



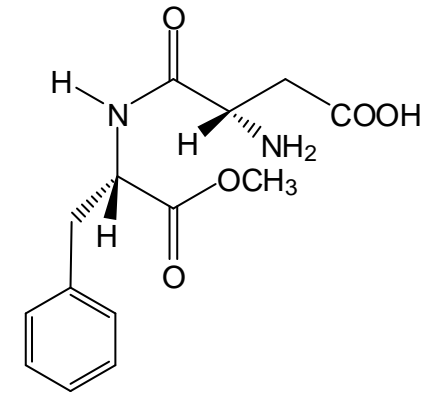
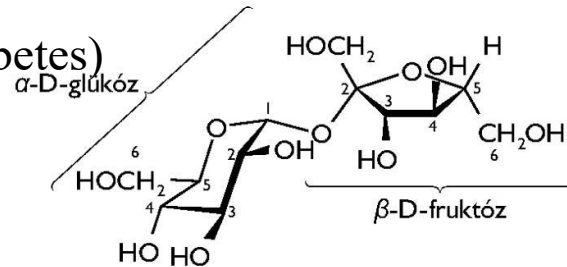
Kockacukor-cukorkocka





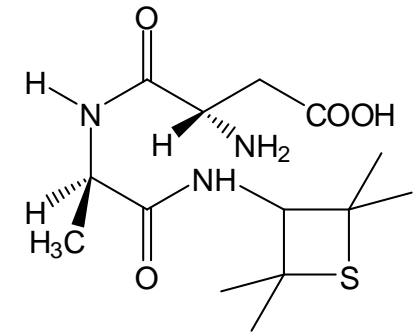
Mesterséges édesítőszer

Alap édesítőszer: szacharóz és a fruktóz
 (kalória túlfogyasztás és fogproblémák, diabetes)
 Megoldás: mesterséges édesítőszer



aszpartám

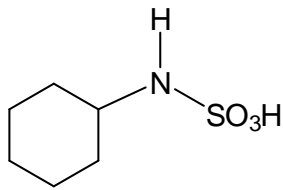
- **Aszpartám** H-Asp-L-Phe-OMe
 (100X édesebb, mint a szacharóz)
 gondok: - lassan hidrolizál (italok)
 - hőre bomlik (sütés)
 - fenilketonureások nem ehetik.



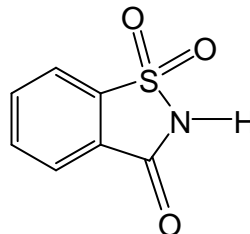
alitám

- **Alitám** (2000X édesebb, mint a szacharóz)
- **Szukralóz:** a szacharóz triklórszármazéka (600X édesebb, mint a szacharóz)
 hőre stabil, fogakat nem bántja

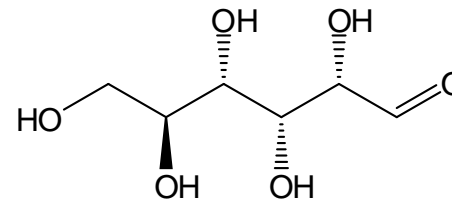
- **ciklamát + szacharin** 10:1 keverék Na^+ vagy Ca^{2+} sói
 - gondok: rákkeltő (betiltva)



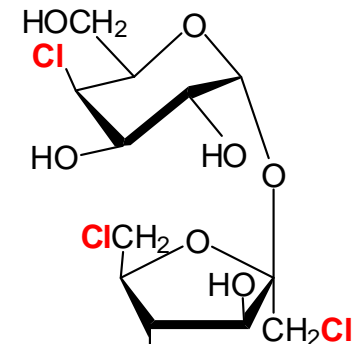
ciklamát



szacharin



L-glükóz

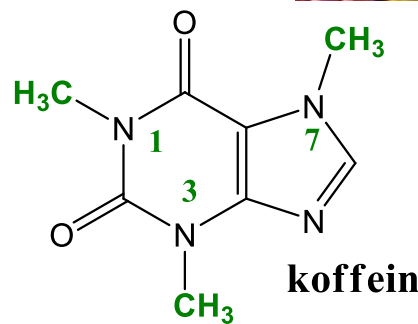
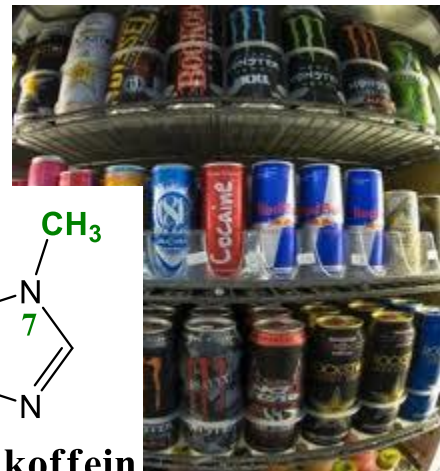
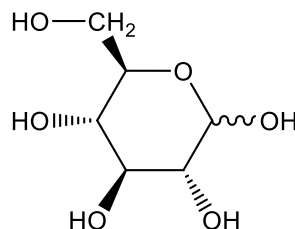
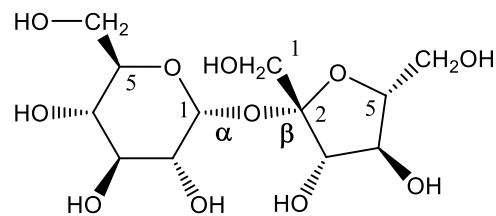


szukralóz

- **L-hexózok** édesek, de nem metabolizálnak,
 viszont drága az előállításuk

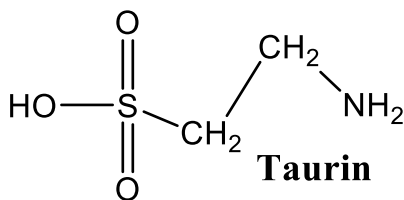
Energiaitalok: az emberi szervezet anyagcseréjét és teljesítőképességét fokozó, ébrenlétet elősegítő üdítőital, összetevők:

- **víz**
- **szénhidrát** (szőlőcukor (D-glükóz) és szacharóz (α -D-Glükózil<1,5>- β -D-fruktozid<2,5>)) gyorsan felszívódó energiaforrás (inzulinszabályozás!)
- **koffein** ~30-35mg/100ml (0,03% ~ **egy dupla** presszókávé)
- **taurin** (0,4%), sejt tápanyagfelvételét fokozó mol.
- savanyú érzetet kontroláló molekulák (**citromsav, nátrium-citrát, magnézium karbonát**)
- vitaminok (nikotinsav (beceneve: **niacin**), **pantoténsav**, B6- és B12-vitaminok)
- íz és látvány „kellékek”



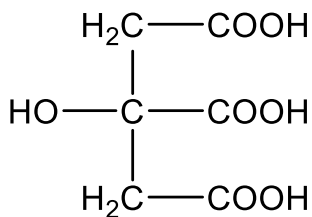
koffein

1,3,7-trimetilxantin

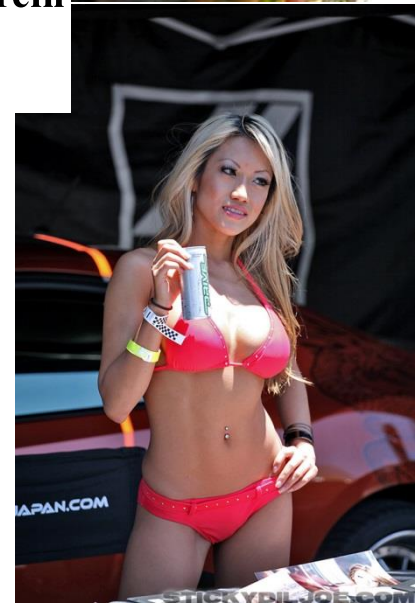


Taurin

2-aminoetán szulfonsav



2-hidroxipropán-
1,2,3-trikarbonsav

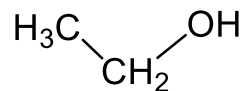


Ellenjavallat:

nem ajánlott: terhes nőknek, szoptató anyáknak, magas vérnyomásban szenvedőknek, szívbetegeknek, koffein érzékeny személyeknek, alkohollal együtt fogyasztva, 14 éven aluli gyermekeknek.

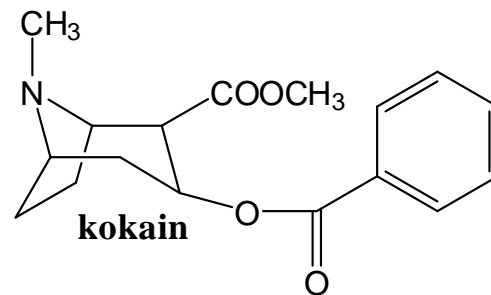
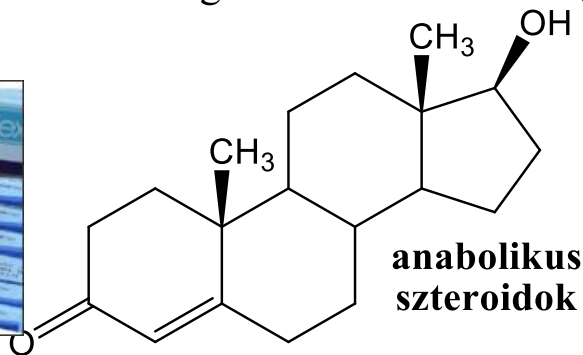
D) Néhány kábítószer:

alkohol

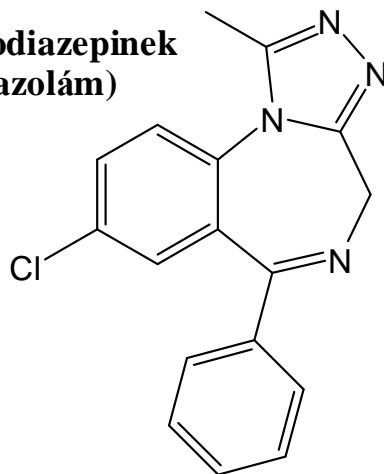


Neurotranszmitterek (pl. GABA) felszabadulását gátolja, módosítja az idegrendszeri Ca^{2+} csatornák működését, fokozza az idegsejtek apoptikus képességét, növeli az idegsej-tmembrán fluiditását, depresszív hatású, metabolitjai (pl. CH_3COH) sejtmérgek, férfiaknál impotenciát okoz (magasabb ösztrogén aktivitás), a prolaktin termelés férfiaknál megnő.

„Az alkohol nem válasz, de elfelejtetted a kérdést!”



benzodiazepinek
(alprazolám)

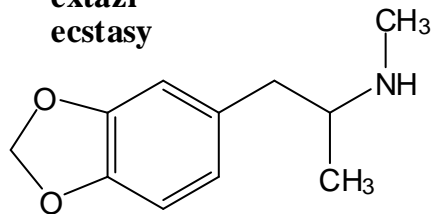


testi hatás: adrenerg receptor stimuláló (vérnyomás fokozó, szívritmus növelő), lassuló emésztés, dehidratáció, **agyi hatás:** (lásd extazi)

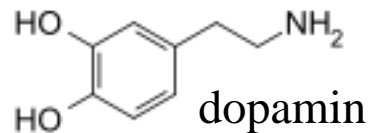
pszichés hatás: kezdetben hangulatjavítás, később agresszivitás, álmatlanság, verejtékezés, impotencia, paranoid viselkedés



**extazi
ecstasy**



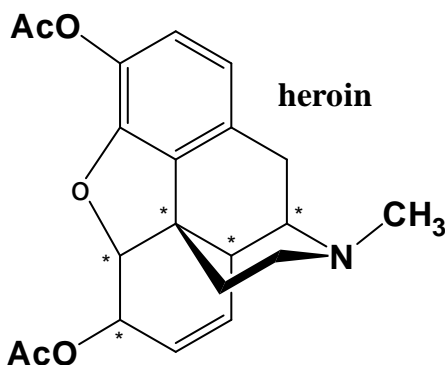
1-(benzo[d][1,3]dioxol-5-yl)-N-methylpropan-2-amine



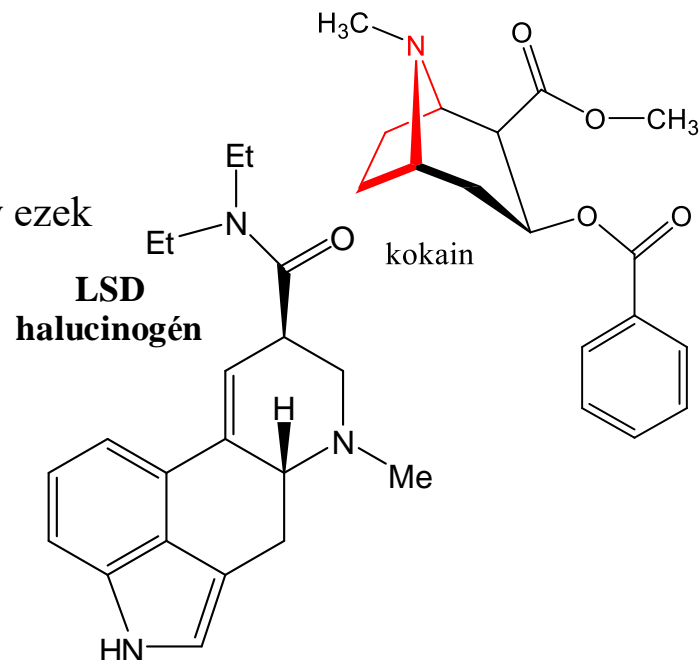
dopamin

Gyorsító (hasonló mint az anfetamin és a kokain)

agyi hatás: akadályozza a noradrenalin, dopamin újrafelvételt, így ezek receptor-stimuláló hatása állandósul



heroin



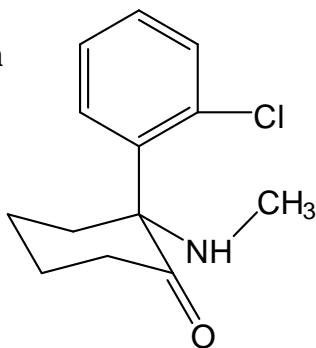
**LSD
halucinogén**

kokain

Depressziót, skizofréniát, pszichózist válthat ki, öngyilkosságba kergethet, halálfélelem, stb.



ketamin

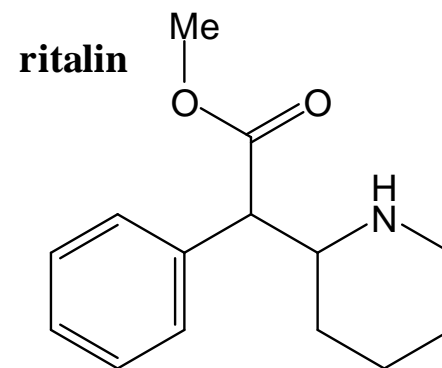
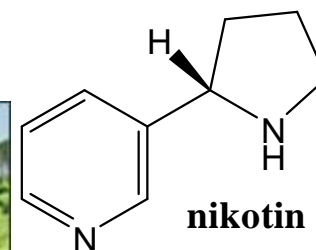
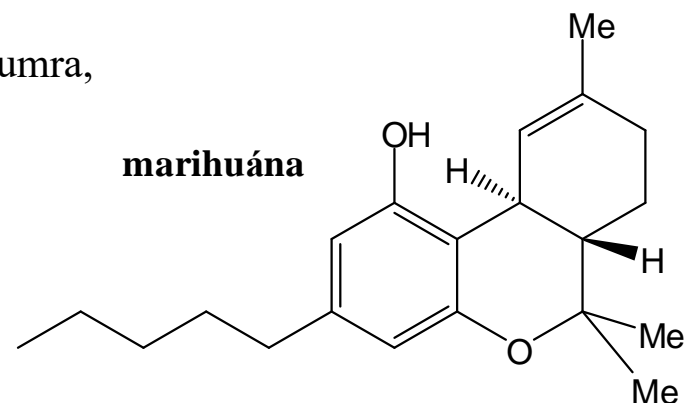


Fájdalomcsillapító hatással rendelkező érzéstelenítő

Mind a központi idegrendszerre (szedatívum) mind a keringésre hat.

Egyetlen cigaretta elszívása (orális bevitel) hat:
a memóriára, a motoros koordinációra (kézremegés), a szenzóriumra,
az idő érzékelésére és a kognitív képességre

Vadkender
(*Cannabis sativa*)



figyelemhiányos hiperaktivitás-
zavar (ADHD) kezelésére
alkalmazzák ~ „gyerek kokain”



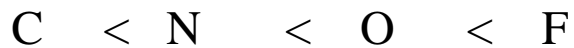
kortex aktiválása
stimuláló hatás
(örökmozgó)

E) Sav-bázis tulajdonságok:

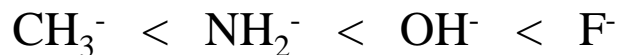
sav-bázis skála:

<i>savasság</i>		<i>bázicitás</i>	pK_a
<i>erős</i>	\uparrow	<i>gyenge</i>	-2.2
	$HCl + H_2O = H_3O^+ + Cl^-$		
	$CH_3SO_3H + H_2O = H_3O^+ + CH_3SO_3^-$		-1.2
<i>gyenge</i>	$HF + H_2O = H_3O^+ + F^-$		+3.2
	$HCOOH + H_2O = H_3O^+ + HCOO^-$		+3.8
	$CH_3COOH + H_2O = H_3O^+ + CH_3COO^-$		+4.7
	$HCN + H_2O = H_3O^+ + CN^-$		+9.2
<i>igen gyenge</i>	$CH_3OH + H_2O = H_3O^+ + CH_3O^-$		+15.5
	$H_2O + H_2O = H_3O^+ + OH^-$		+15.7
	$NH_3 + H_2O = H_3O^+ + NH_2^-$	<i>erős</i>	+33
<i>nem</i>	$CH_4 + H_2O = H_3O^+ + CH_3^-$		>40

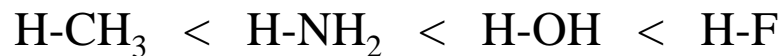
A) az elektronegativitás mint a savasság mértékét befolyásoló tényező



—————→ elektronegativitás nő



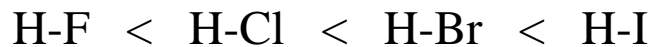
—————→ stabilitás nő



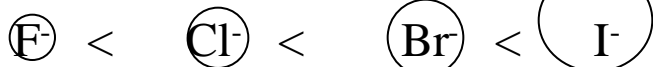
—————→ savas karakter nő

B) a konjugált bázis mérete

mint a savasság mértékét befolyásoló tényező

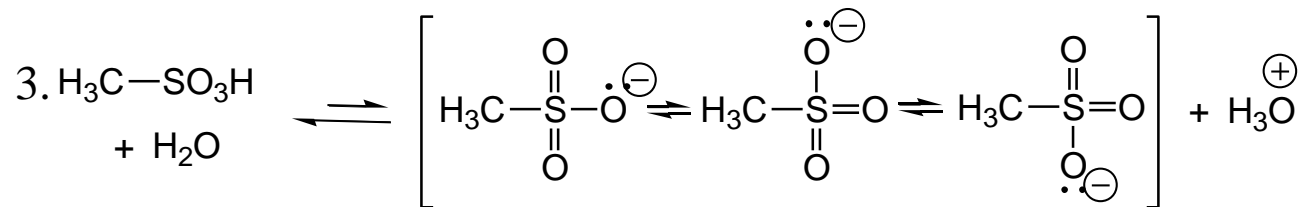
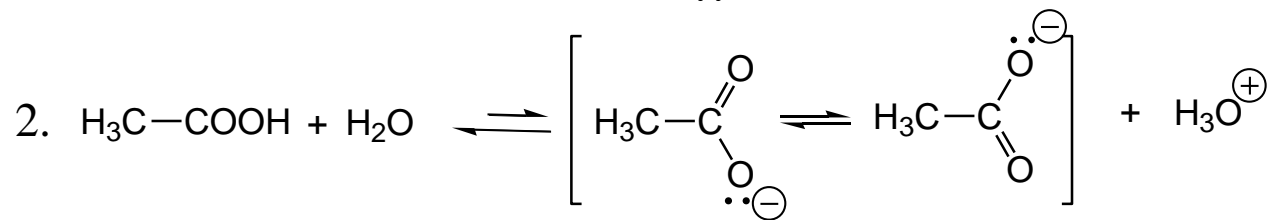
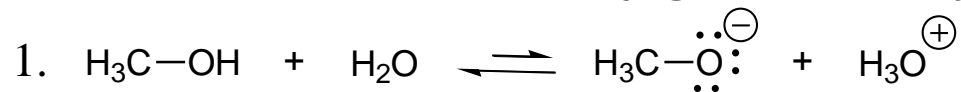


—————→ savas karakter nő



—————→ a konjugált bázis mérete nő

C) sav-bázis rendszerekben a **konjugáció** stabilizálja a konjugált bázist




1. nincs konjugáció → $\text{pK}_a \sim 16$

2. van konjugáció → $\text{pK}_a \sim 5$

3. van konjugáció → $\text{pK}_a \sim 1$

finomhangolás I:

A) az alifás lánchossz hatása karbonsavak esetén	pK_a
H-COOH	3.75
CH ₃ -COOH	4.74
CH ₃ -(CH ₂) ₁ -COOH	4.87
.	
.	
.	
CH ₃ -(CH ₂) ₈ -COOH	4.84
B) az alifás lánchossz hatása alkoholok esetén	pK_a
„H-OH”	„15.7”
CH ₃ -OH	15.5
CH ₃ -(CH ₂) ₁ -OH	15.9
ⁱ Pr-OH	16.5
^t Bu-OH	18.0
 -OH	18.0

konklúzió: Az alkil-lánc hosszának növekedésével a savas karakter csökken, mivel a konjugált bázis hidratálhatósága egyre gyengébb.

memo: Az alkil-csoport elektron küldő hatása tovább csökkenti a sav savi jellegét.

finomhangolás II:

A. elektronvonzó csoport hatása alifás karbonsavak esetén:

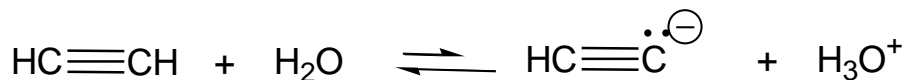
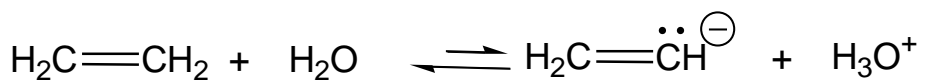
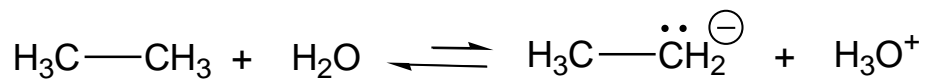
		pK_a
H-CH ₂ -COOH		4.74
I-CH ₂ -COOH		3.18
Br-CH ₂ -COOH		2.90
Cl-CH ₂ -COOH		2.86
F-CH ₂ -COOH	elektronszívó csoport	2.59
Cl ₂ C-COOH	HALOGÉN	1.26
Cl ₃ C-COOH		0.64
F ₃ C-COOH		0.23

CH ₂ =CH-CH ₂ -COOH	elektronszívó csoport	4.35
N≡C-CH ₂ -COOH	EGYÉB	2.46
NO ₂ -CH ₂ -COOH		1.68

B. elektron szívó csoport hatása alifás alkoholok esetén:

	pK_a
H-CH ₂ -CH ₂ -OH	15.9
Cl-CH ₂ -CH ₂ -OH	14.3
CCl ₃ -CH ₂ -OH	12.2

memo: C-savak savas karaktere



pK_a	C hibr.	S-kar.
50	sp^3	~25%
44	sp^2	~33%
25	sp	~50%

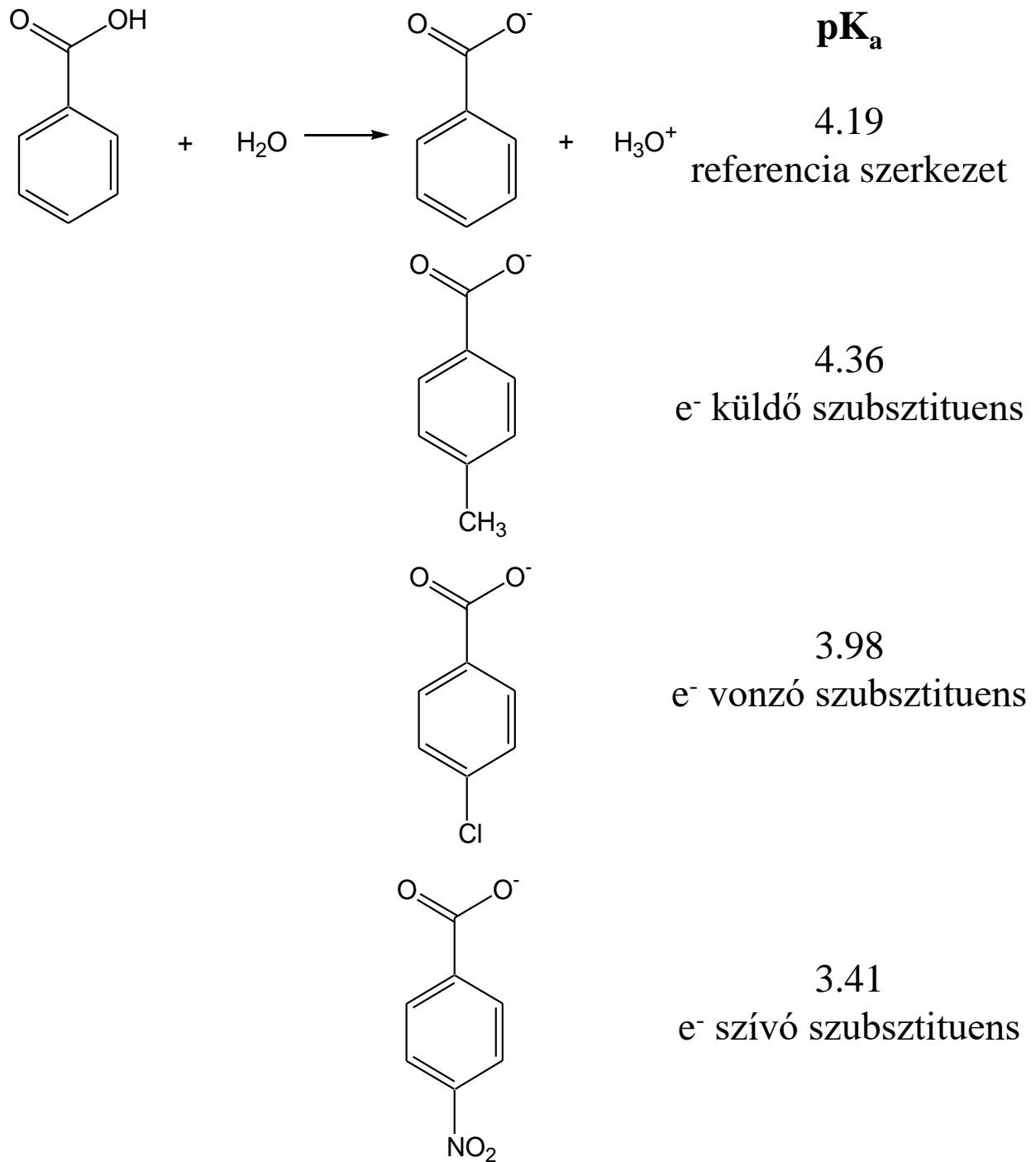
memo: ammónia

alifás alkohol

33

16-18

finomhangolás III:



memo:

Ha a sav-bázis pár savi részében fokozott az elektronelszívás, az deformálja az aromás rendszer elektroneloszlását.

A savasságot fokozza a konjugált bázis szolvatálhatóságának növekedése.

Összefoglaló (fontosabb fogalmak)

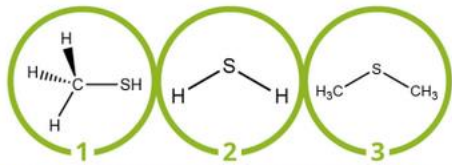
- heterociklusos szénvegyületek aromás jellege
- apoláris és poláris határszerkezetek (pl. pirrol, indolát anion,
- tautomerek (barbitursav, uracil,
- nukleinsavak építőelemei
- Watson-Crick bázispárok molekulaszervezete
- a DNS RNS kémiai szervezete

THE CHEMISTRY OF BODY ODOURS

BODY ODOURS ARE COMMONLY THE RESULT OF BACTERIAL ACTIVITY - FOR EXAMPLE, BACTERIA LIVING ON OUR SKIN BREAK DOWN THE SECRETIONS OF SWEAT INTO ODOUROUS COMPOUNDS. THIS GRAPHIC SHOWS THE MAIN COMPOUNDS RESPONSIBLE FOR PARTICULAR ODOURS.

rossz
szájszag

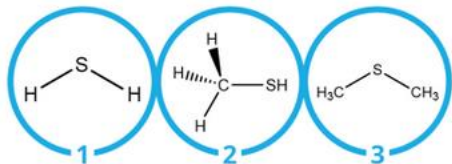
HALITOSIS



NAME	SMELLS LIKE
1. METHANETHIOL	sulfur, garlic
2. HYDROGEN SULFIDE	sulfur, rotting eggs
3. DIMETHYL SULFIDE	cabbage, sulfur, sweet

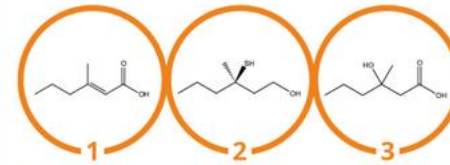
felfúvódás

FLATULENCE



NAME	SMELLS LIKE
1. HYDROGEN SULFIDE	sulfur, rotting eggs
2. METHANETHIOL	sulfur, garlic
3. DIMETHYL SULFIDE	cabbage, sulfur, sweet

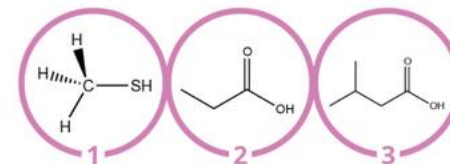
UNDERARM ODOUR



NAME	SMELLS LIKE
1. (E)-3-METHYL-2-HEXENOIC ACID	goat
2. (S)-3-METHYL-3-SULFANYLHEXAN-1-OL	onion
3. 3-HYDROXY-3-METHYLHEXANOIC ACID	cumin

hónalj
szag

FOOT ODOUR



NAME	SMELLS LIKE
1. METHANETHIOL	sulfur, garlic
2. PROPANOIC ACID	pungent, rancid, sour
3. ISOVALERIC ACID	cheesy, fermented, rancid

láb
szag