

NBCM-010

# Bioorganická chemie

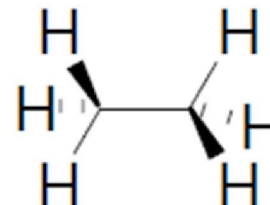
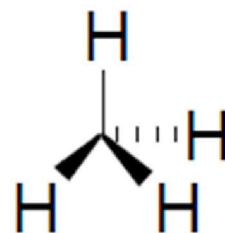
Cvičení – konformace CIP pravidla

Kateřina Hofbauerová

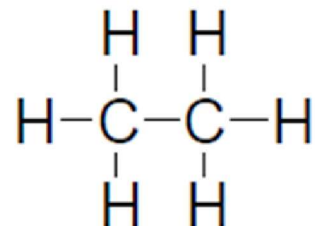
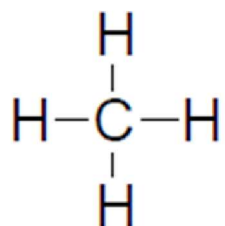


vzorce

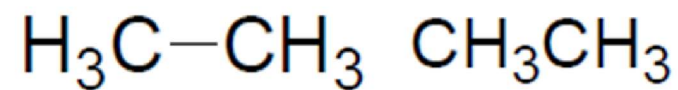
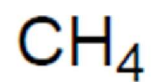
perspektivní



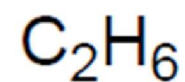
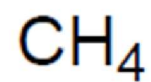
strukturní

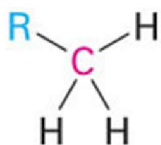


zjednodušené strukturní



souhrnné (sumární)





**Primary carbon (1°)**  
is bonded to one  
other carbon.

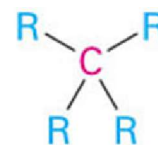
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**Secondary carbon (2°)**  
is bonded to two  
other carbons.



**Tertiary carbon (3°)**  
is bonded to three  
other carbons.



**Quaternary carbon (4°)**  
is bonded to four  
other carbons.

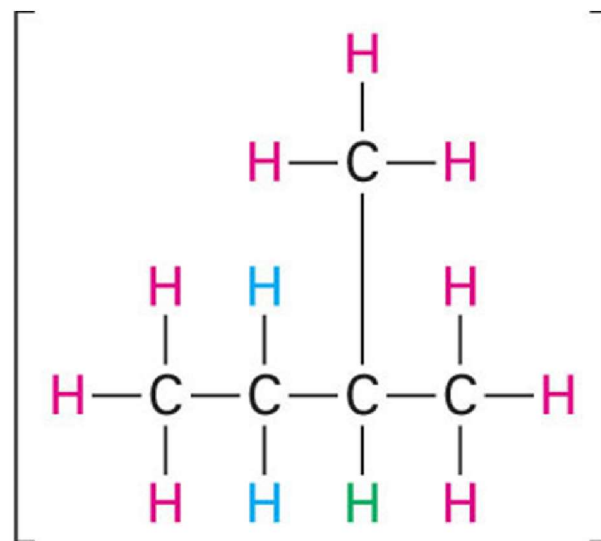
Primary hydrogens (CH<sub>3</sub>)



Secondary hydrogens (CH<sub>2</sub>)

A tertiary hydrogen (CH)

=



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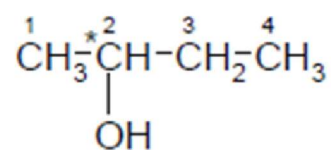
## CIP pravidla

Robert Sidney Cahn (1899-1981), Sir Christopher Ingold (1893-1970) a Vladimir Prelog (1906-1998)

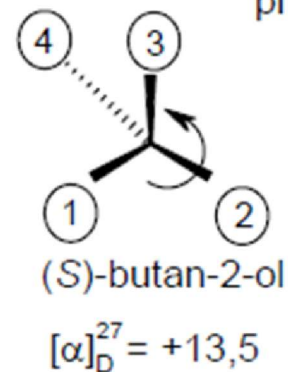
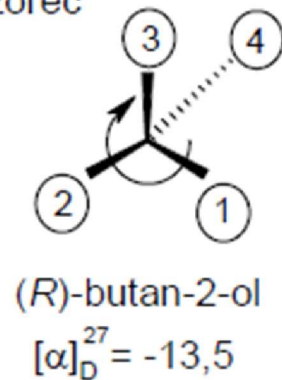
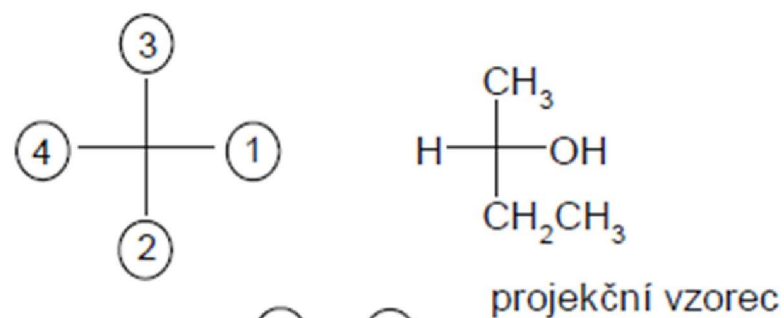
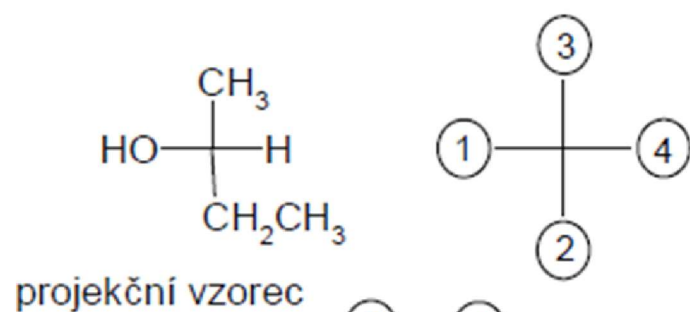
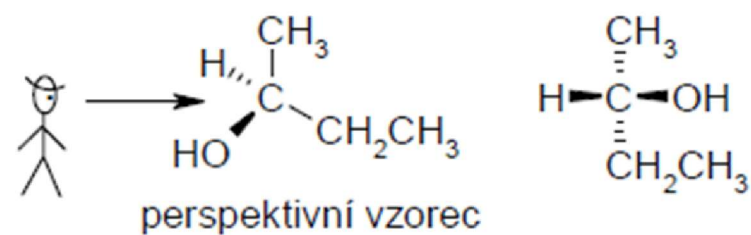
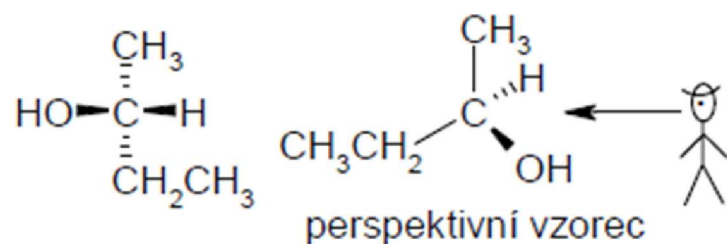
Pravidlo posloupnosti představuje způsob, jakým se určuje nadřazenost skupin, substituentů i ligandů kolem stereogenního centra. V prvním přiblížení postačí pořadí podle klesajících protonových čísel atomů bezprostředně k němu vázaných, např.  $\text{Cl} > \text{S} > \text{F} > \text{O} > \text{N} > \text{C}$ ; podobně se pokračuje v dalším přiblížení, např.  $\text{CH}_2\text{Cl} > \text{CH}_2\text{OH} > \text{CH}_2\text{CH}_3 > \text{CH}_3$ . Substituent má se přiřadit číslo v pořadí klesající priority, tedy v pořadí **1** > **2** > **3** > **4**, kde symbol > znamená, že je nadřazen. ve smyslu pravidla posloupnosti. V případě butan-2-olu tak bude hydroxyskupina náležet **1**, ethylu **2**, methylu **3** a vodíkovému atomu **4**.

Smysl chiralit - absolutní konfigurace se poté odvozuje podle druhého pravidla, které definuje směr otáčení pomyslného volantu, a to ve směru klesající priority zbývajících substituentů (**1** **2** **3**). Otáčí-li se pomyslným volantem doprava, přiřazuje se stereogennímu centru ( $\text{C}^*$ ) stereodeskriptor (symbol, afix) **R** (lat. *rectus*, pravý), otáčí-li se doleva, přiřazuje se afix **S** (lat. *sinister*, levý). V názvech sloučenin se afixy **R** a **S** píšou kurzivou, umísťují se v závorkách před úplný název sloučeniny, od něho. Se oddělují spojovníkem.

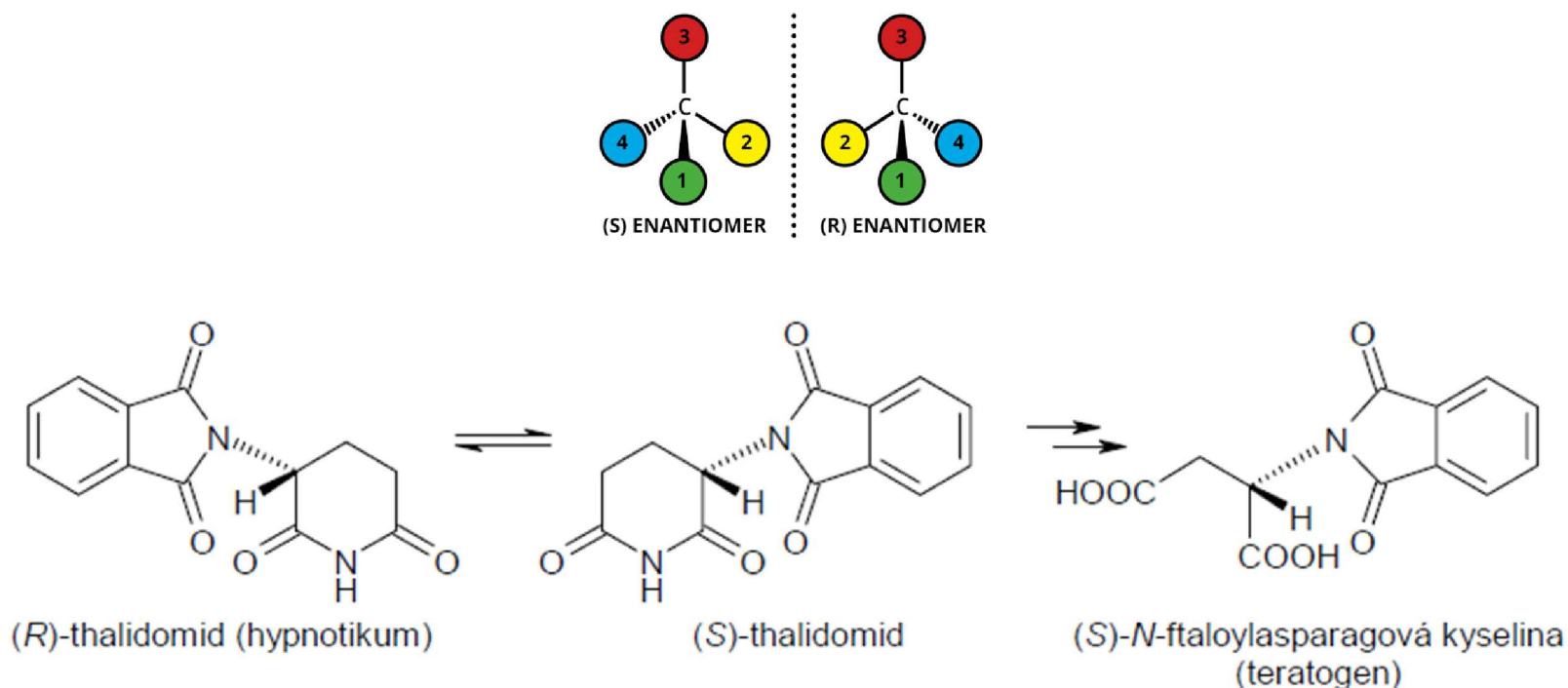
Ekvimolární směs pár enantiomerů (1:1) se nazývá racemát.



konstituční vzorec

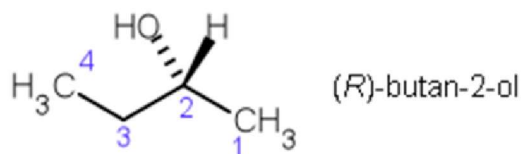


zrcadlová rovina

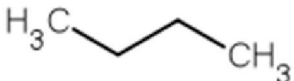
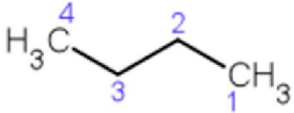
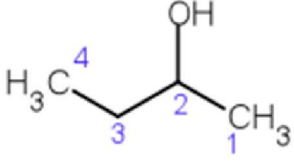
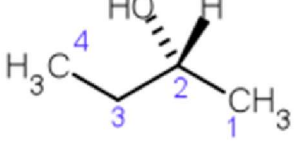


**(S)-thalidomid** je p vodcem primárn znetvo ení paží mezi 40. až 44. dnem embryonálního vývoje, dále pak i dolních kon etin mezi 43. až 46. dnem – teratogen, respektive jeho metabolický produkt.  
**(R)-thalidomid** p sobí proti ranním nevolnostem

## (R)-butan-2-ol

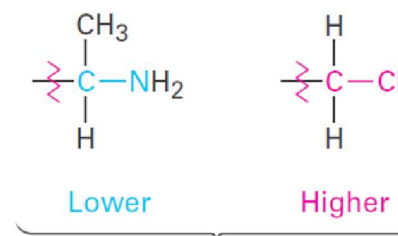
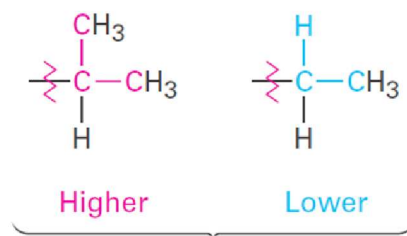
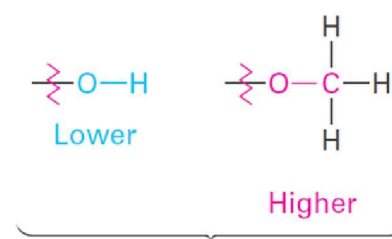
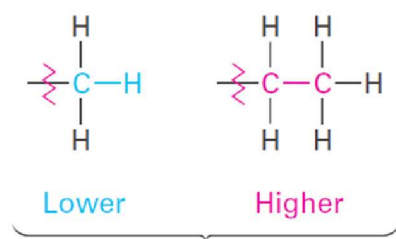


### Postup převodu názvu na strukturu

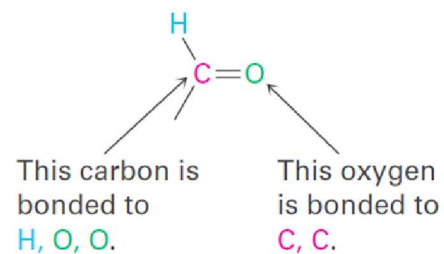
Struktura	Název	Poznámka
	butan	<i>Základ názvu</i>
		<i>Číslování</i>
	butan-2-ol	
	(R)-butan-2-ol	<i>Kompletní struktura</i>

Substituent m se p i adí ísla v po adí klesající priority, tedy v po adí **1** > **2** > **3** > **4**, kde symbol > znamená, že je nad azen, ve smyslu pravidla posloupnosti. V p ípad butan-2-olu tak bude hydroxyskupin náležet **1**, ethylu **2**, methylu **3** a vodíkovému atomu **4**.

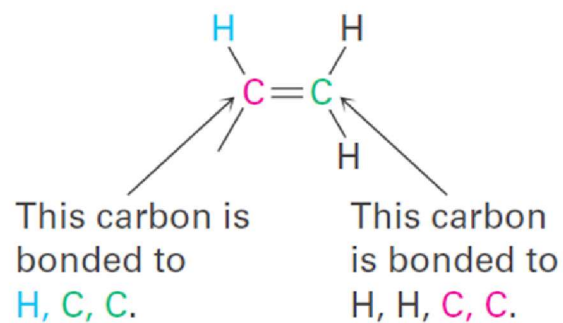
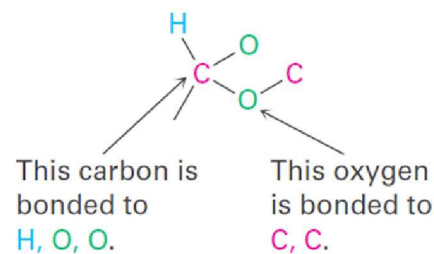
**Atomic number**    35    17    16    15    8    7    6    (2)    (1)  
**Higher ranking**   Br > Cl > S > P > O > N > C > <sup>2</sup>H > <sup>1</sup>H    **Lower ranking**



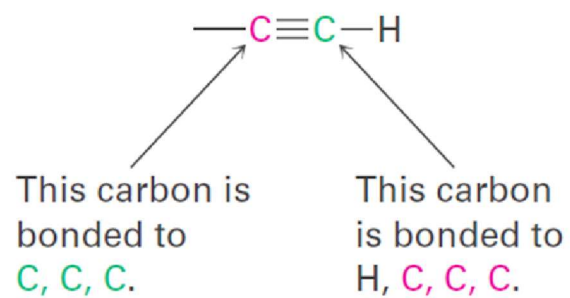
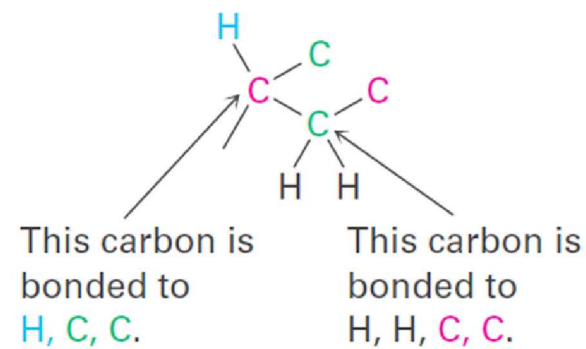




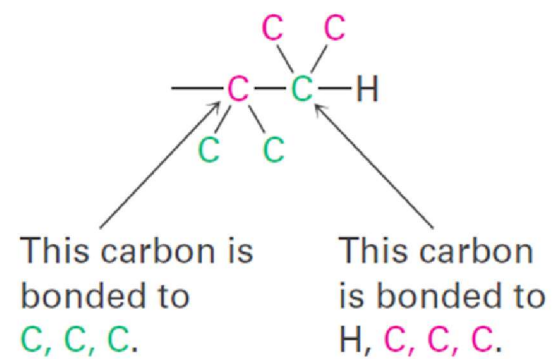
is equivalent to

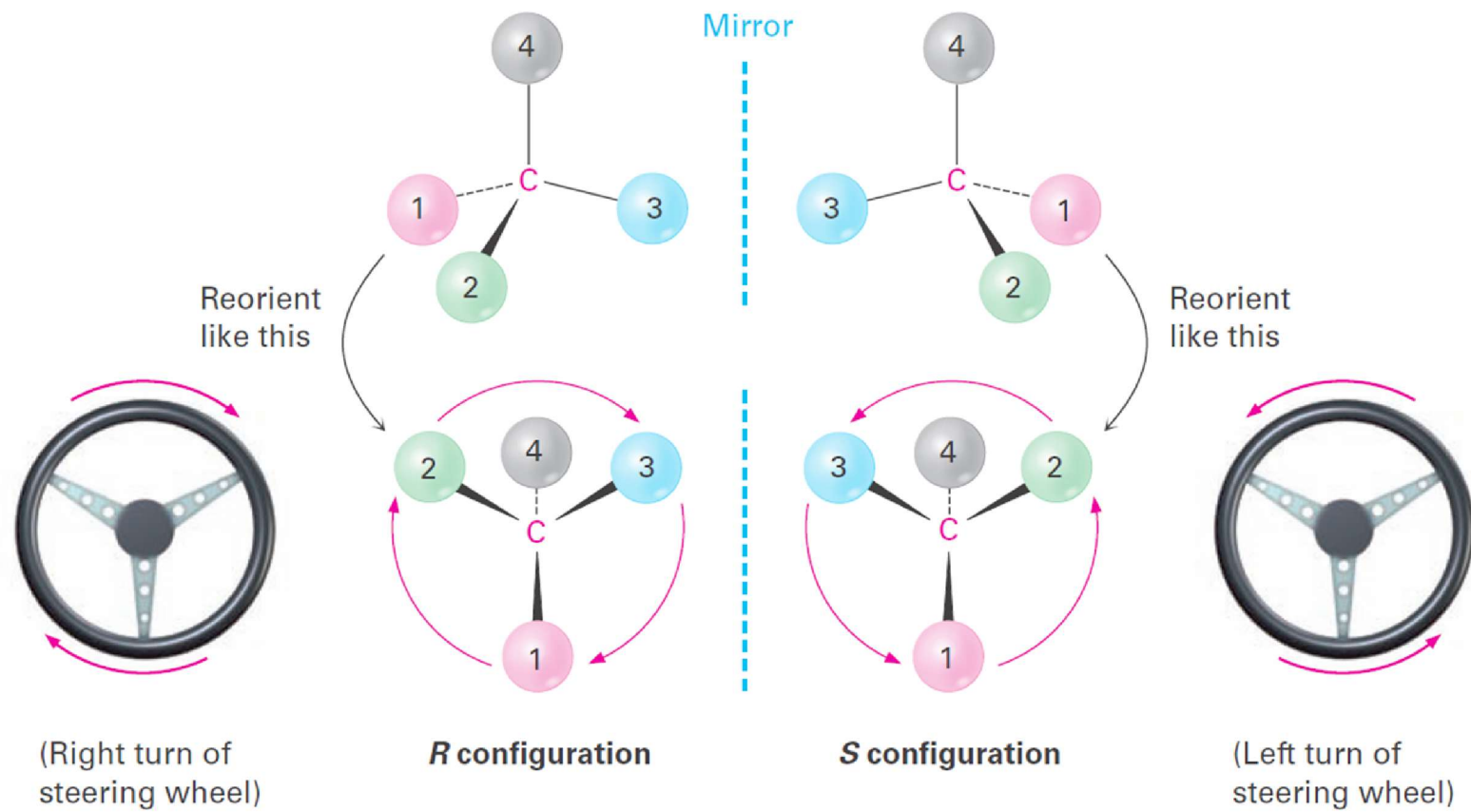


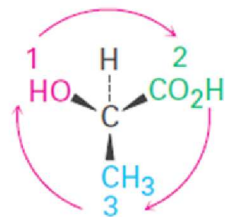
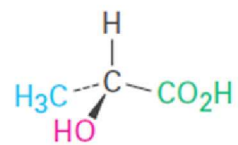
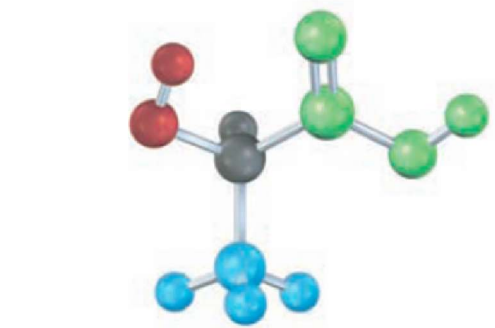
is equivalent to



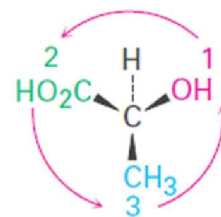
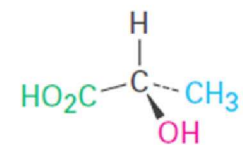
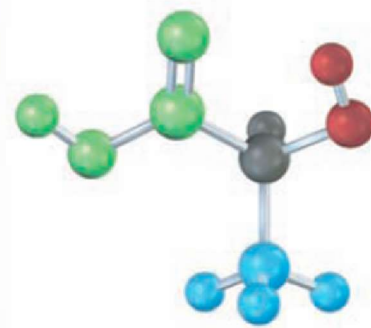
is equivalent to



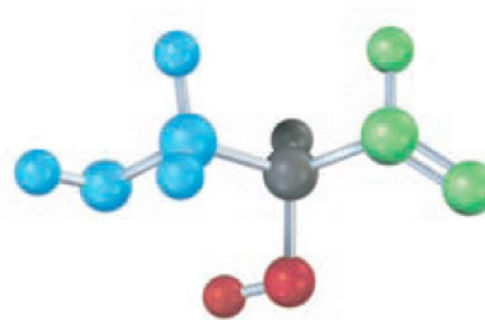
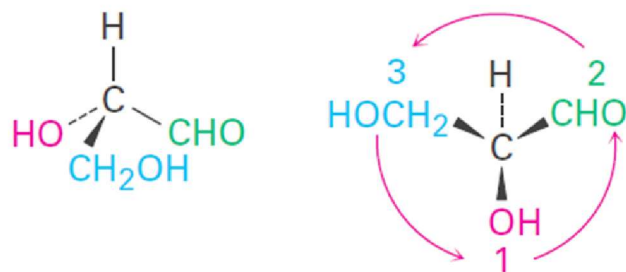




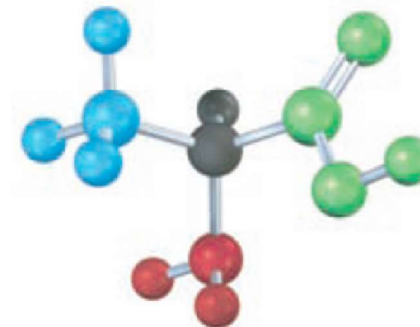
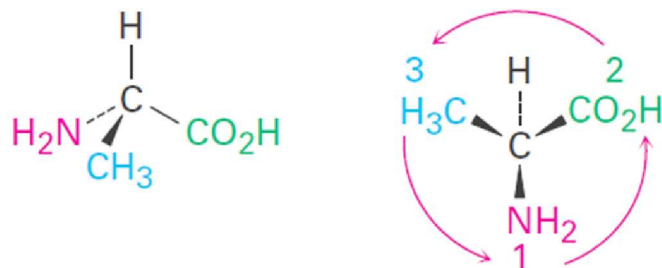
***R* configuration**  
(*R*)-(-)-lactic acid



***S* configuration**  
(*S*)-(+)-lactic acid

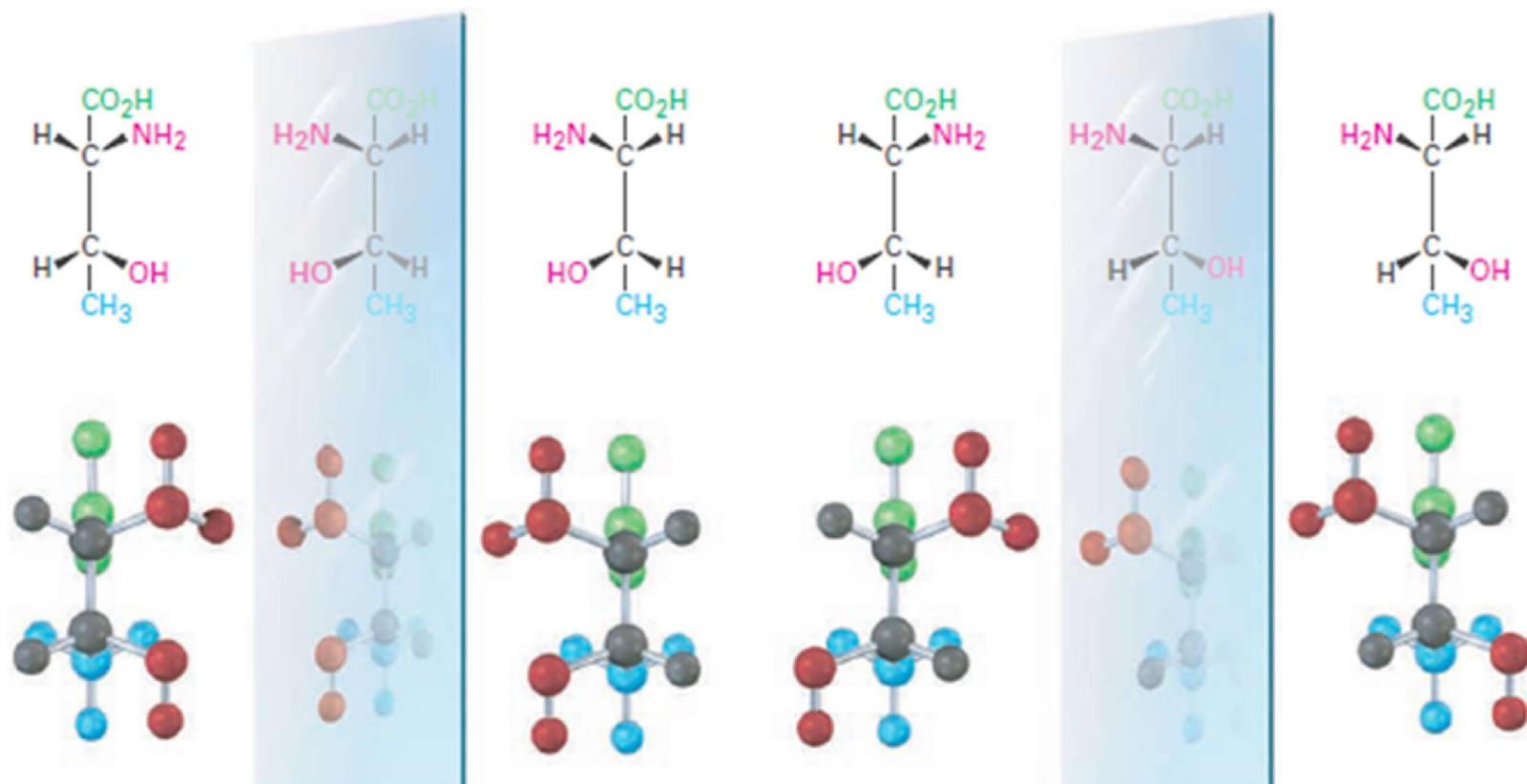


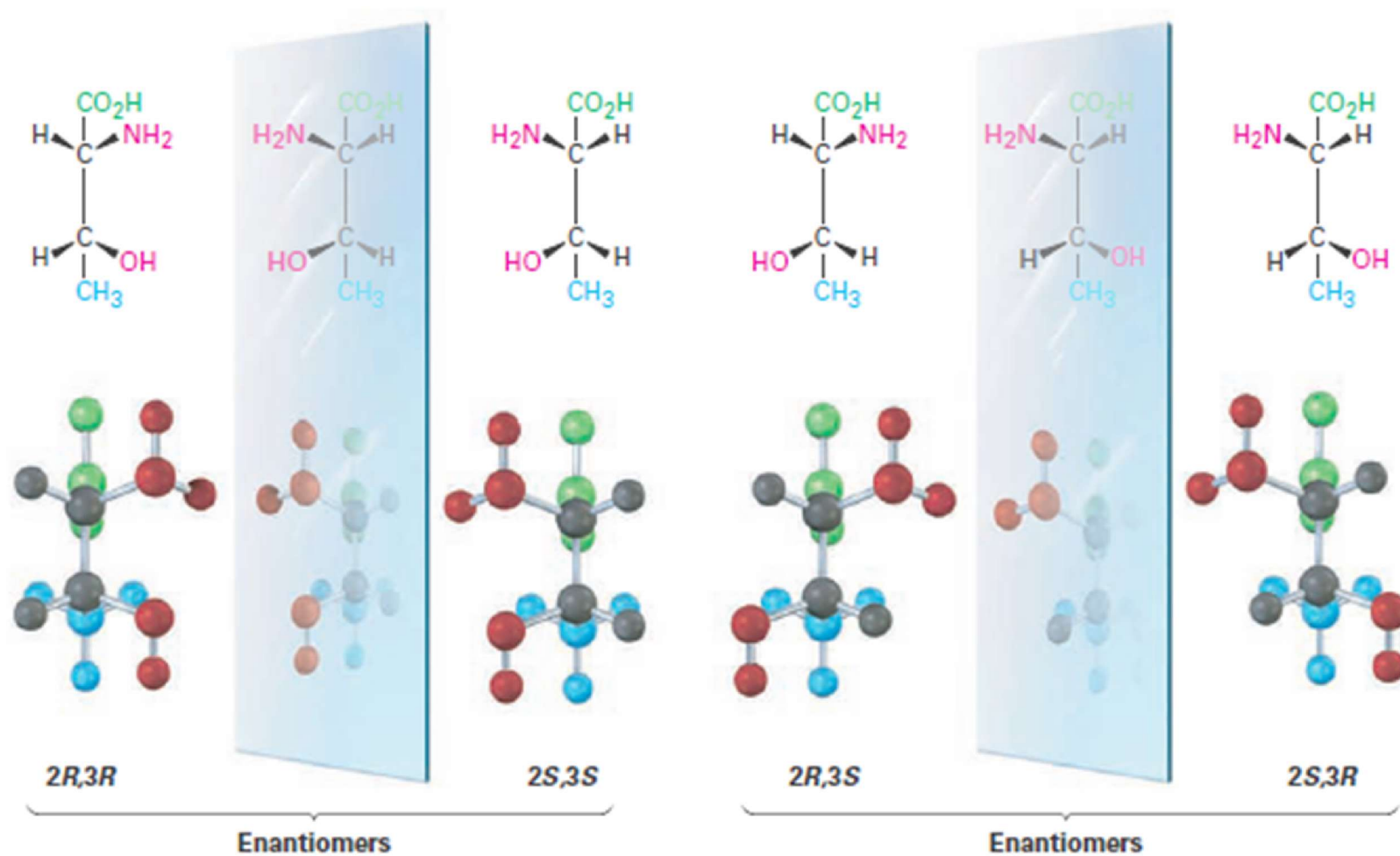
**(S)-Glyceraldehyde**  
**[(S)-(-)-2,3-Dihydroxypropanal]**  
 $[\alpha]_D = -8.7$



**(S)-Alanine**  
**[(S)-(+)-2-Aminopropanoic acid]**  
 $[\alpha]_D = +8.5$

Ur ete absolutní konfiguraci





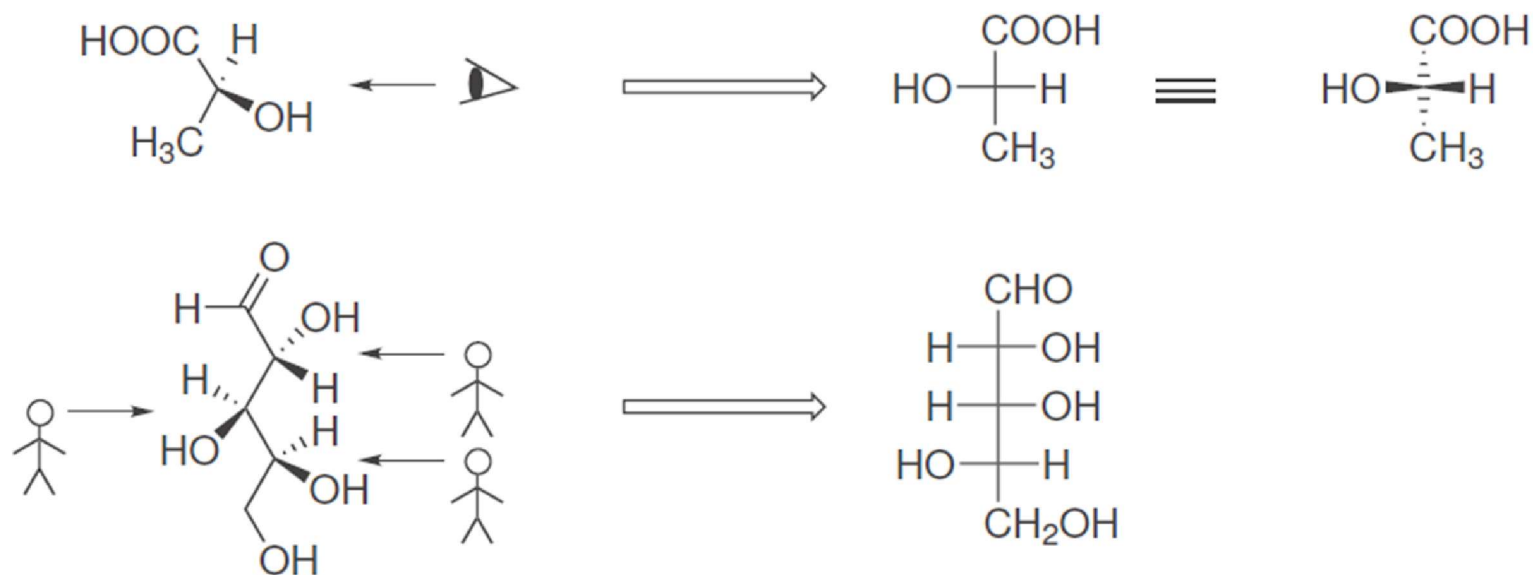
**FIGURE 5.10** The four stereoisomers of 2-amino-3-hydroxybutanoic acid.

2-amino-3-hydroxybutanová kyselina

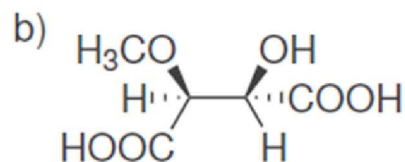
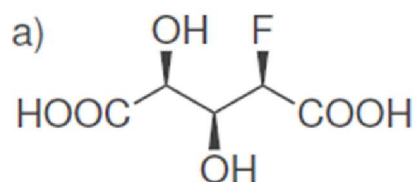
Aminokyselina threonin - (2S,3R)-2-amino-3-hydroxybutanová kyselina

# Fischerova projekce

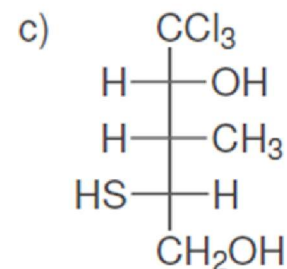
Nejčastěji je používána pro znázornění prostorového uspořádání sacharidů a podobných derivátů.



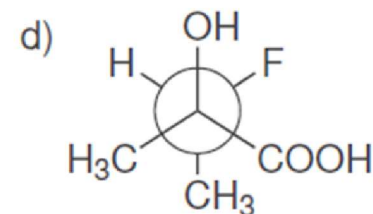
# Pojmenujte sloučeniny, určete absolutní konfiguraci a převeďte z jednoho nebo do Fischerovy projekce



klínkové  
zobrazení



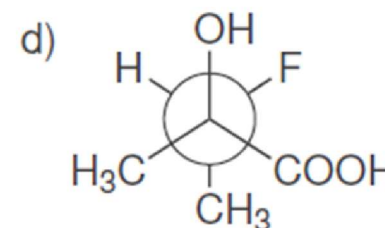
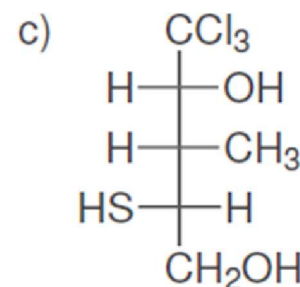
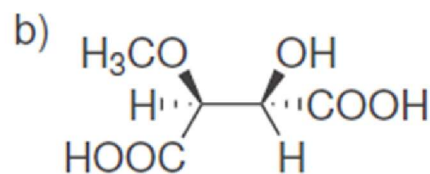
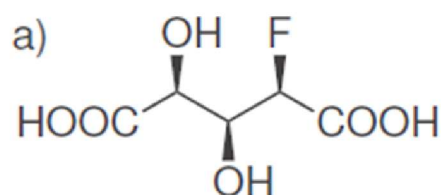
Fischerova  
projekce



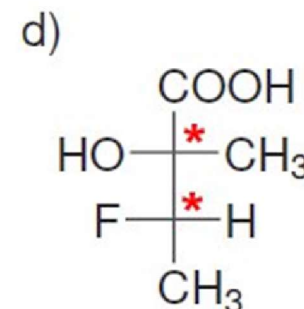
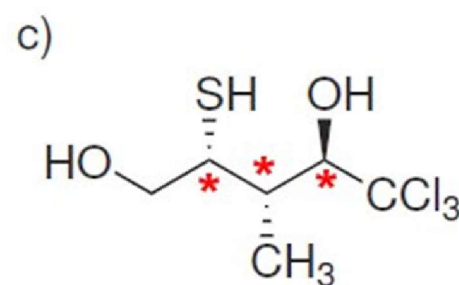
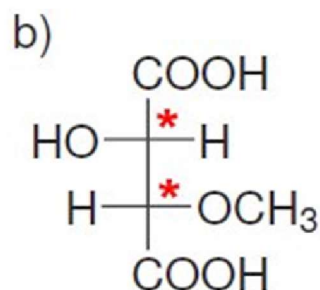
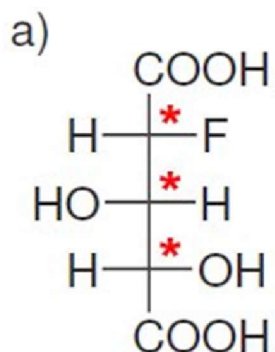
Newmanova  
projekce



# Pojmenujte sloučeniny, určete absolutní konfiguraci a převeďte z nebo do Fischerovy projekce

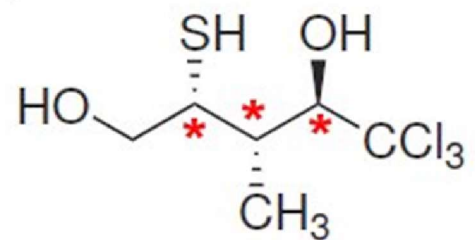


Zobrazení v projekci a označení stereogenních center

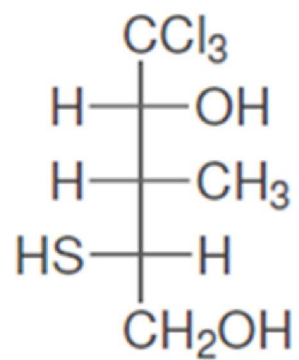
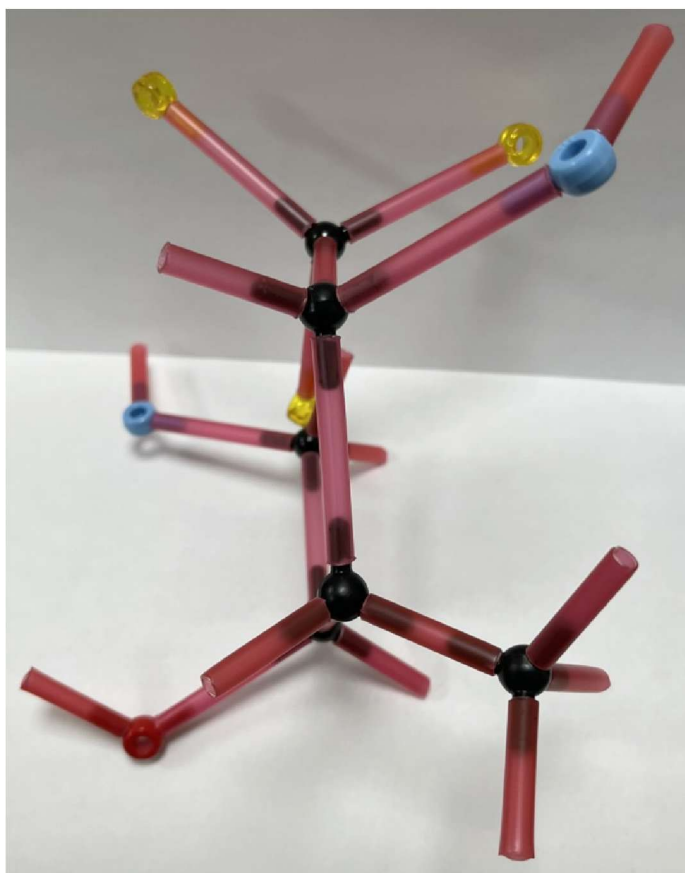


Po adí d ležitosti podle protonových čísel  
 $\text{Cl } 17 > \text{S } 16 > \text{F } 9 > \text{O } 8 > \text{N } 7 > \text{C } 6 > \text{H } 1$

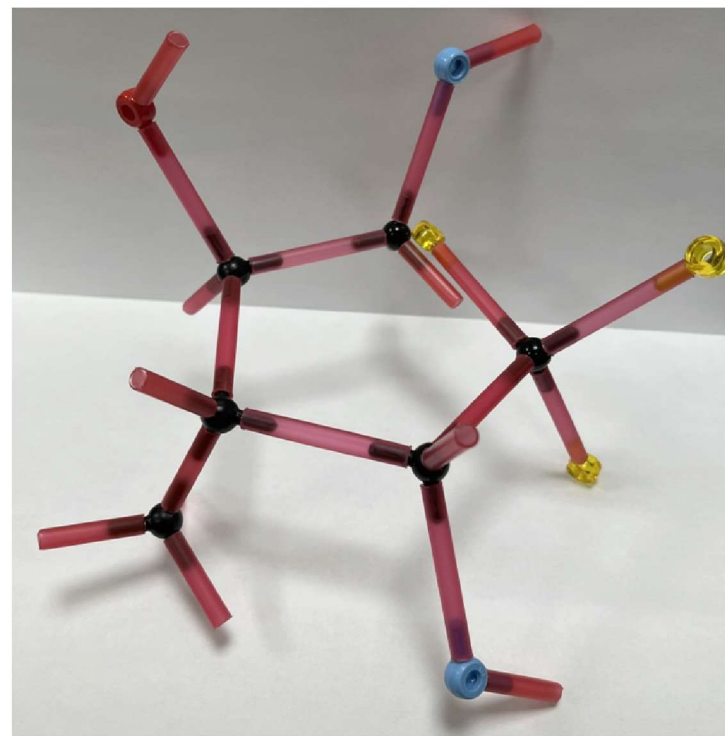
c)



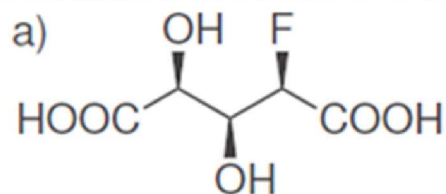
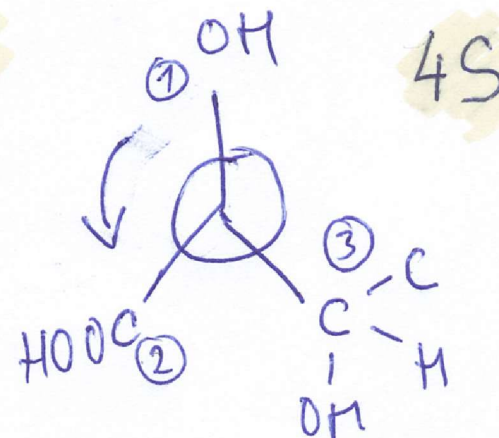
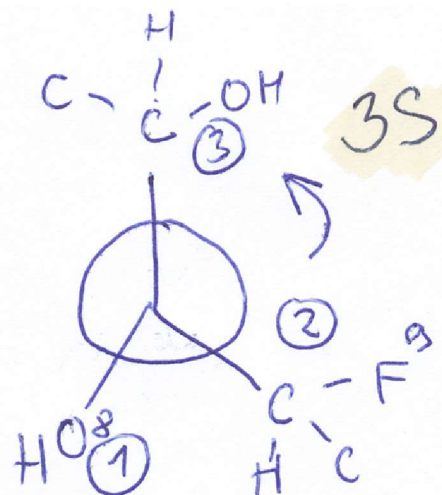
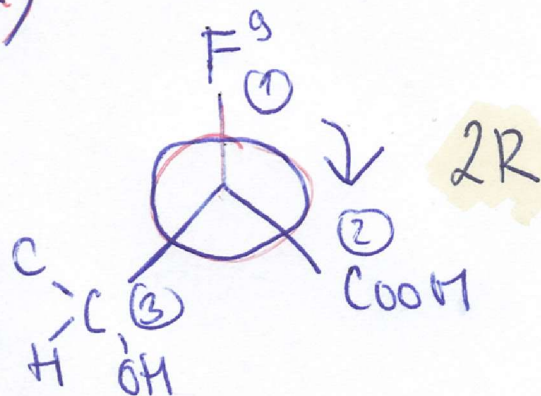
Místo vodík jsou na fotografii kratší vazby, kyslík je modré, chlor žlutý, síra červená



Fisherova projekce

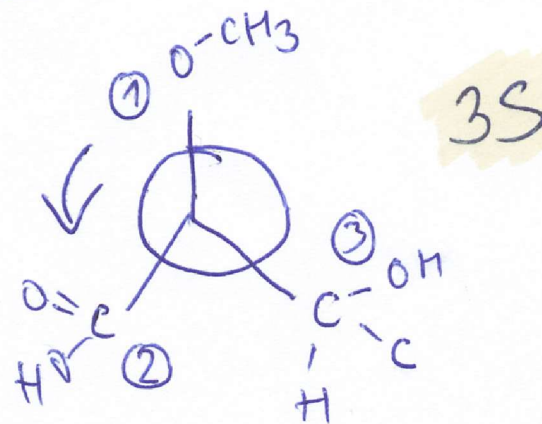
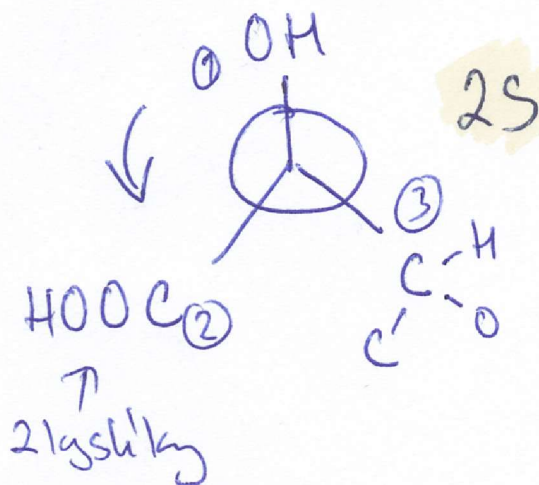
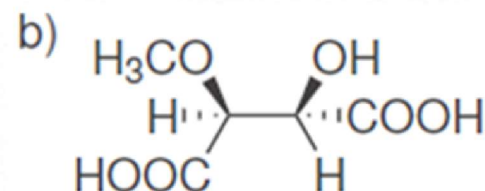


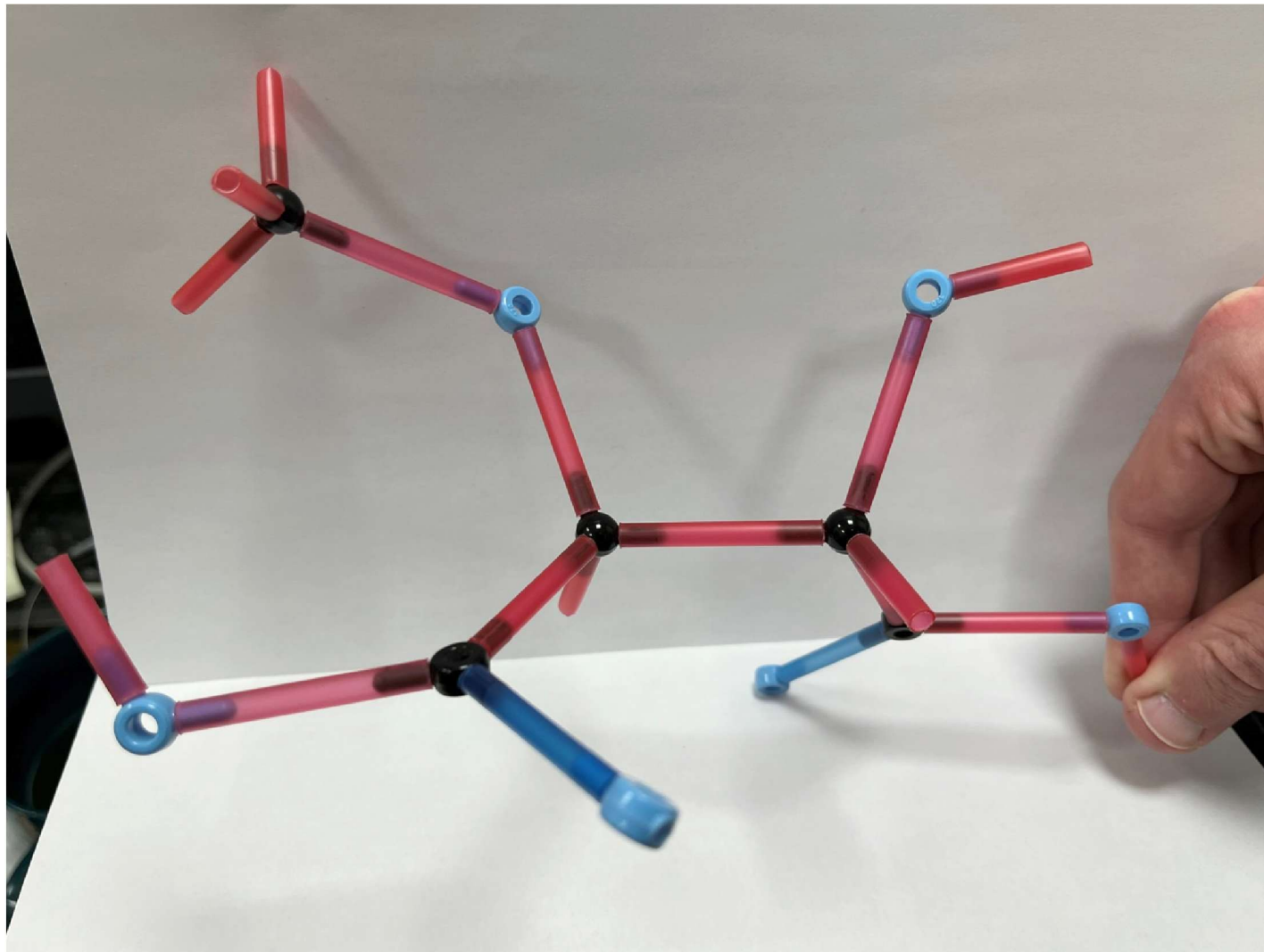
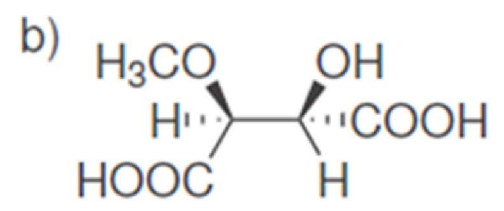
a)



vodík do začnu

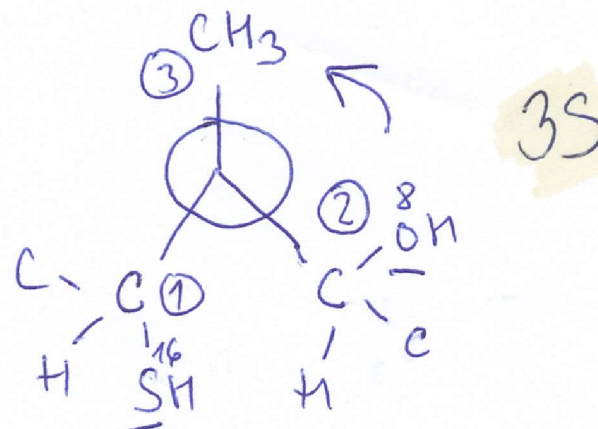
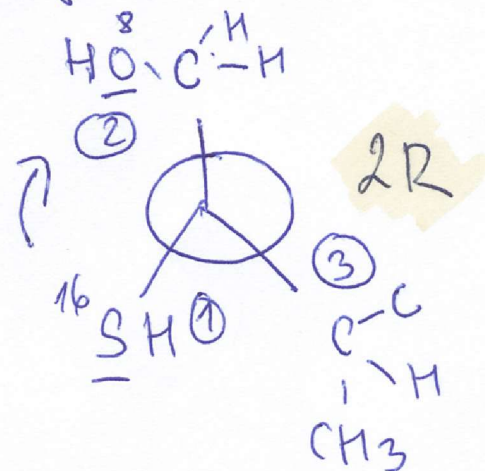
b) pro pozici 2 v původním zobrazení  
skóit molekulu; H sněitije pod plochu



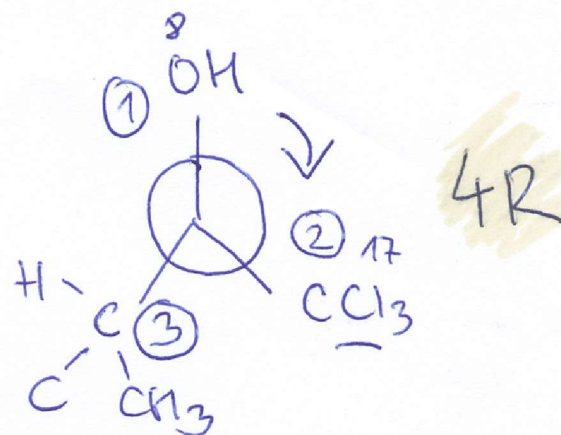
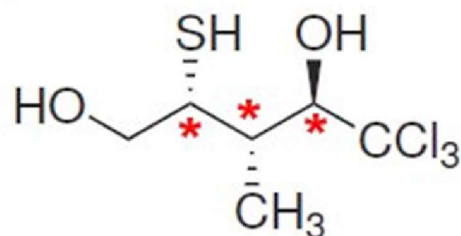


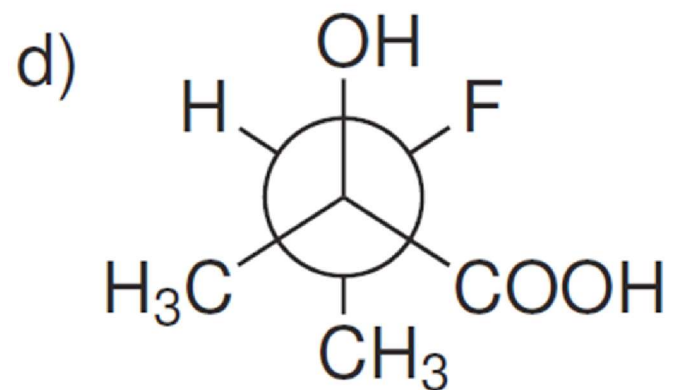


c) pro pozici 2 a 3 stereochemický molekulu; H směřuje pod plochu

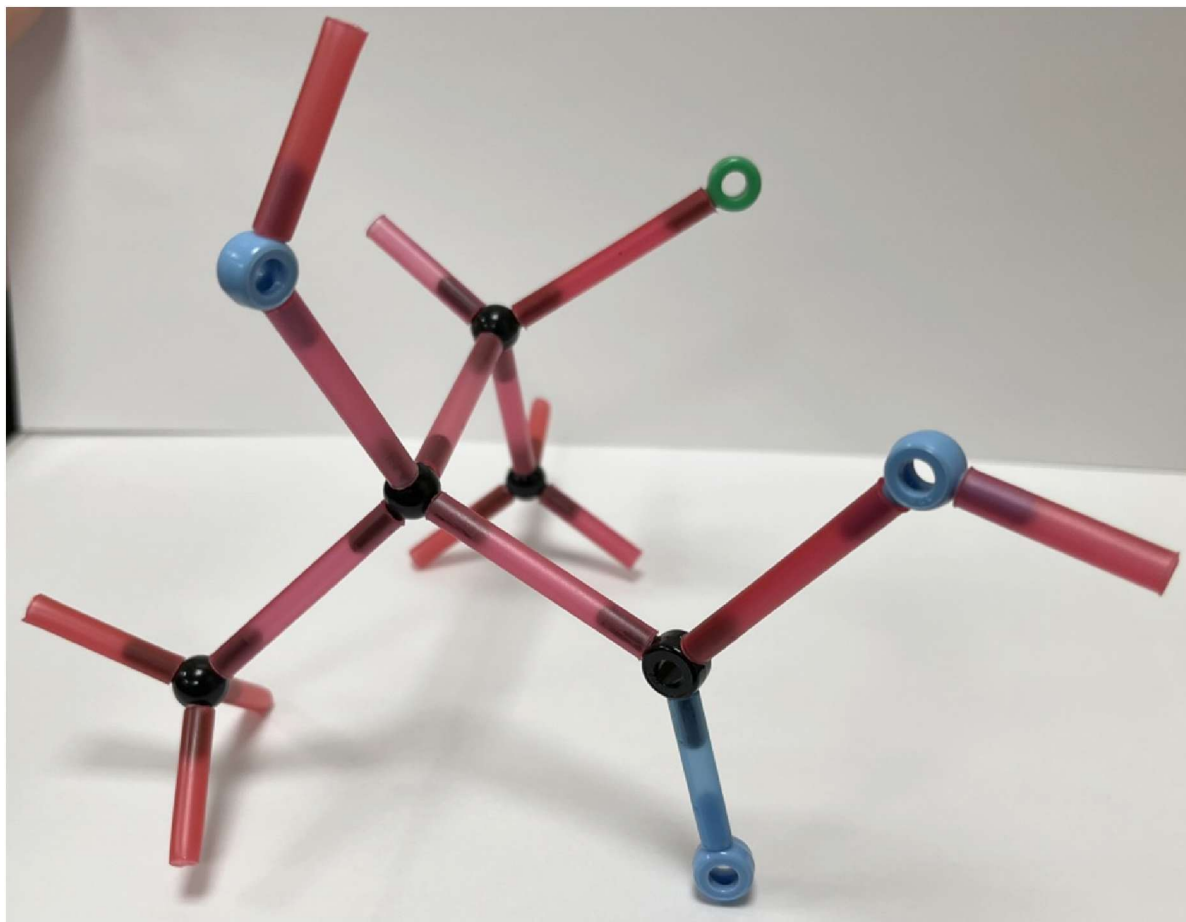


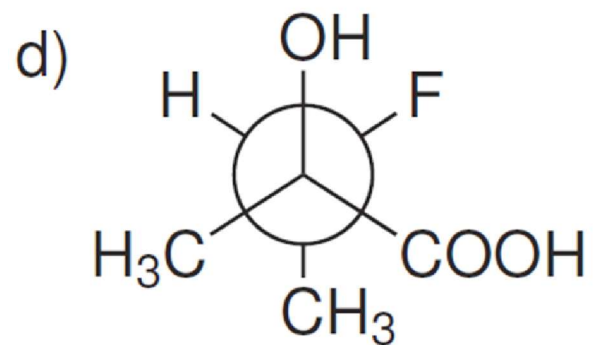
c)



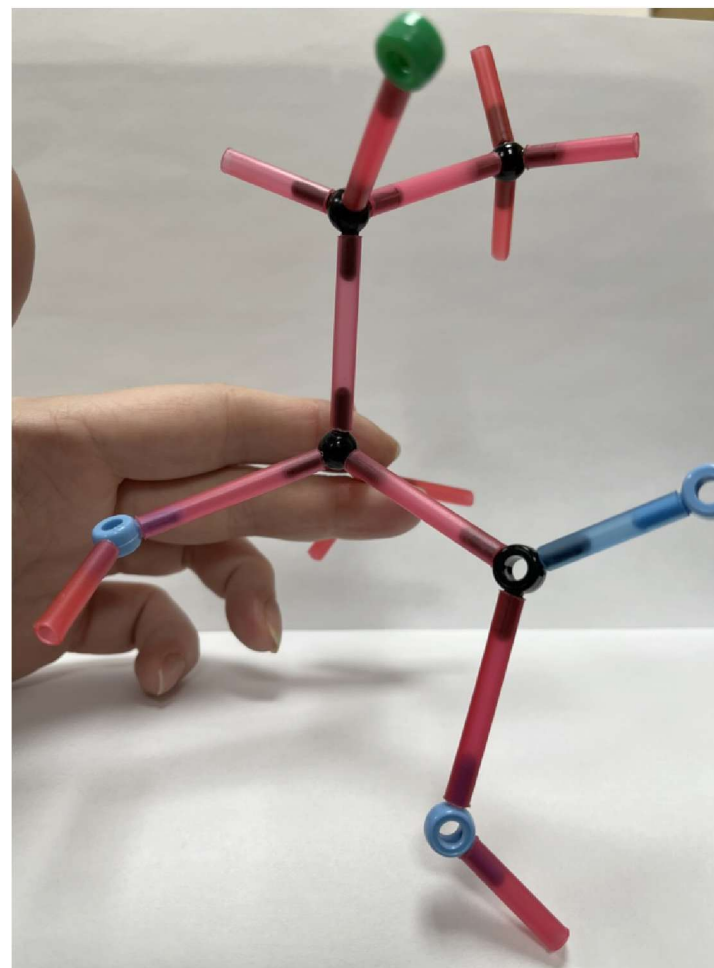
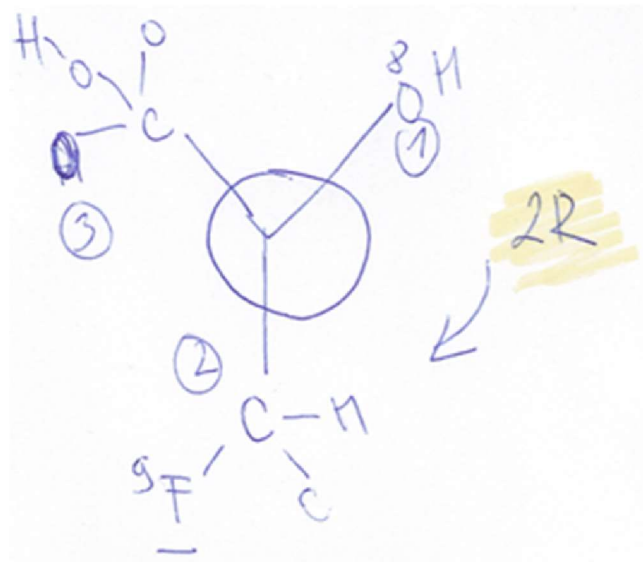


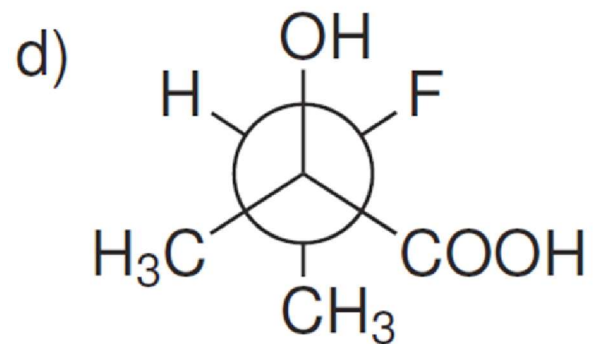
Místo vodík jsou na fotografii kratší vazby, kyslík je modré, fluor zelený, dvojná vazba modré



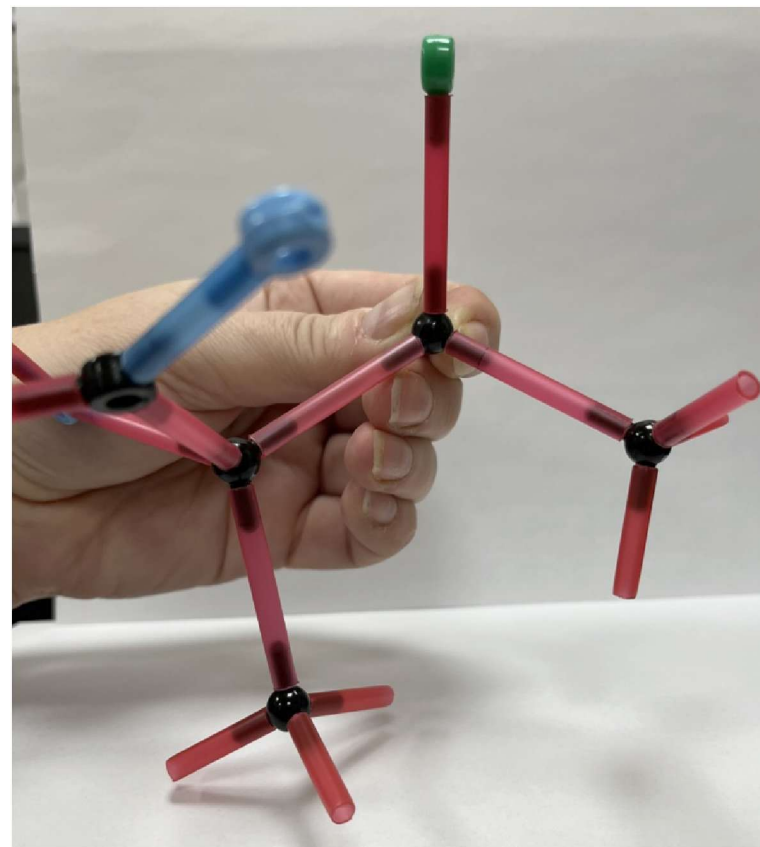
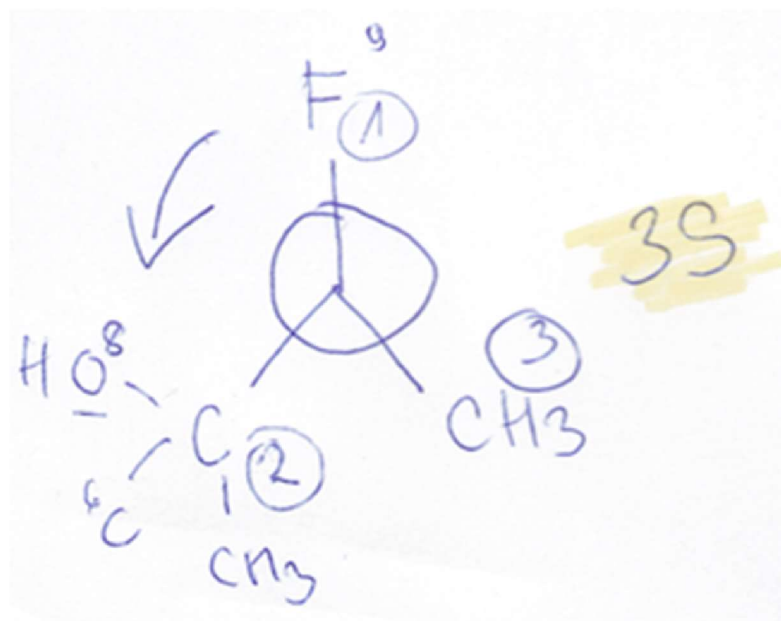


Místo vodík jsou na fotografii kratší vazby, kyslík je modré, fluor zelený, dvojná vazba modrá



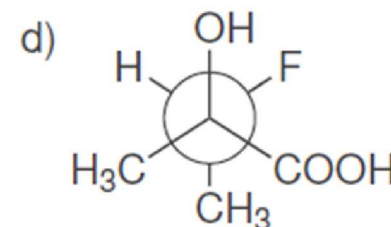
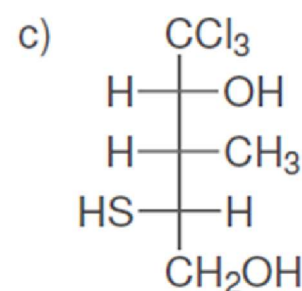
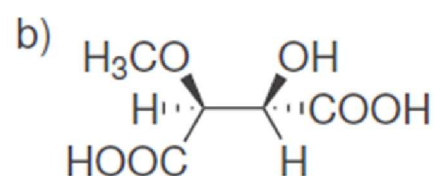
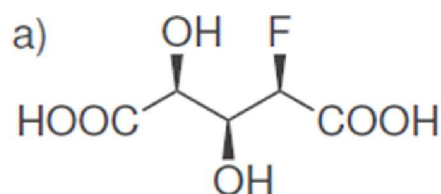


Místo vodík jsou na fotografii kratší vazby, kyslík je modré, fluor zelený, dvojná vazba modré



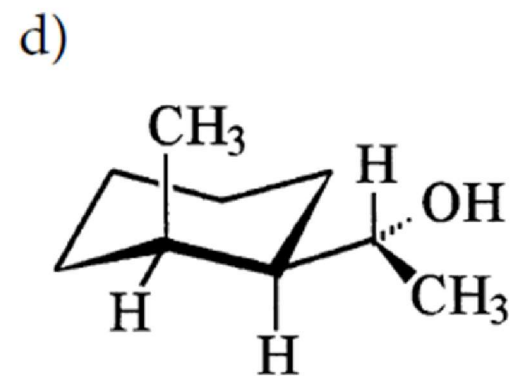
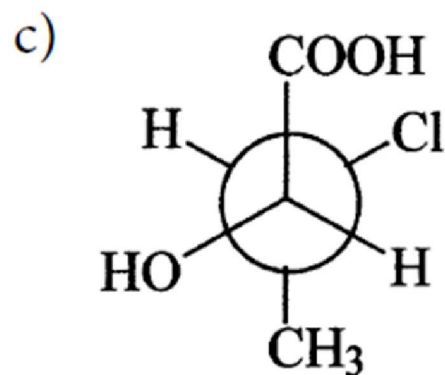
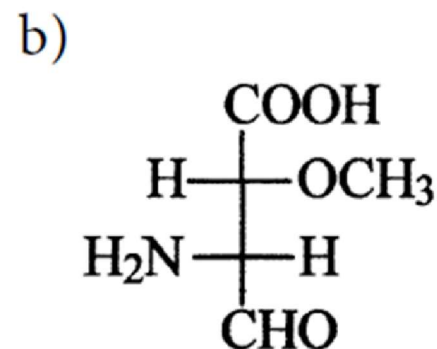
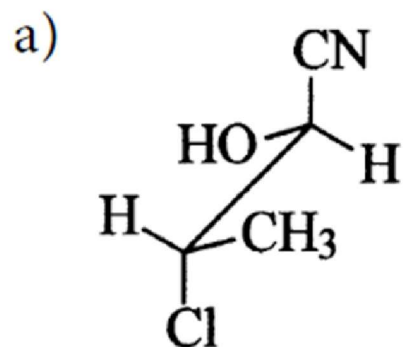


# Pojmenujte sloučeniny, určete absolutní konfiguraci a převeďte z nebo do Fischerovy projekce



- (a) (2R,3S,4S)-2-fluor-3,4-dihydroxypentan-1,5-diová kyselina  
 (b) (2S,3S)-2-hydroxy-3-methoxybutan-1,4-butandiová kyselina  
 (c) (2R,3S,4R)-5,5,5-trichlor-3-methyl-2-sulfanylpentan-1,4-diol  
 (d) (2R,3S)-3-fluor-2-hydroxy-2-methylbutanová kyselina

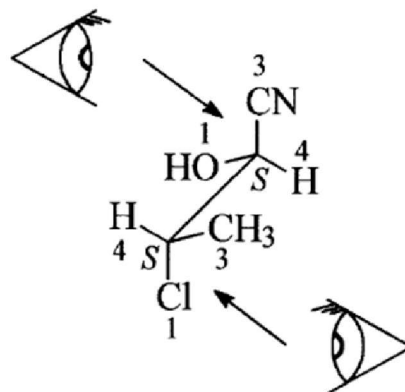
# Určete absolutní konfiguraci sloučenin



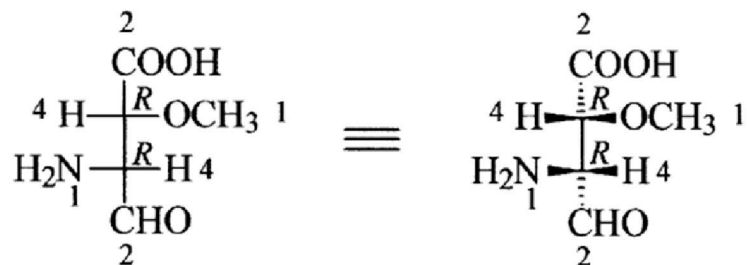
Newmanova projekce

# Určete absolutní konfiguraci sloučenin

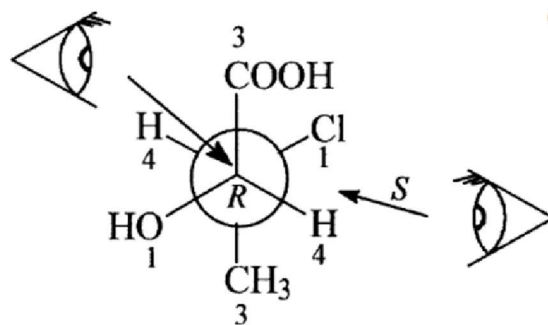
a)



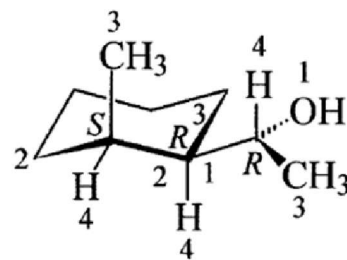
b)



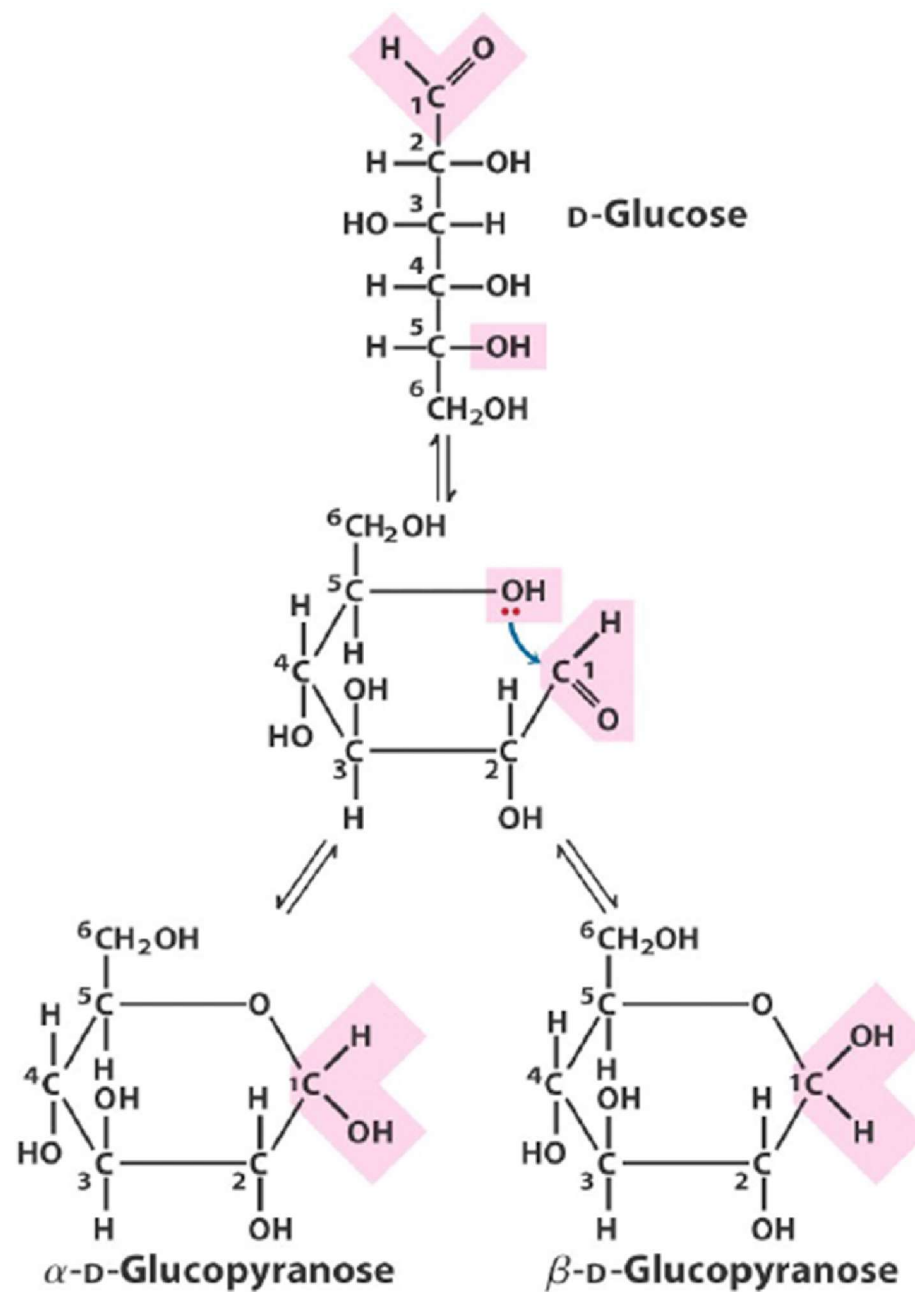
c)



d)

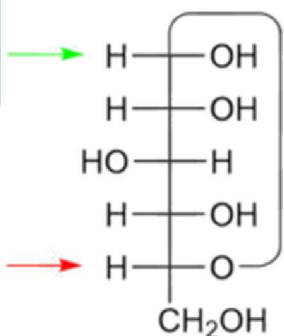
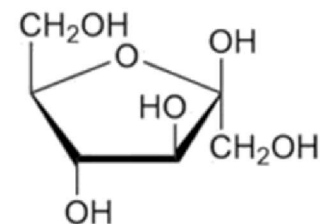
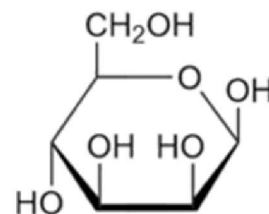
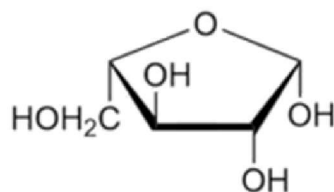
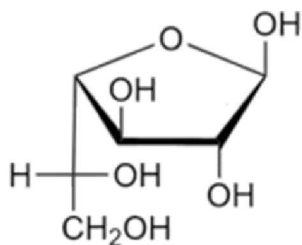
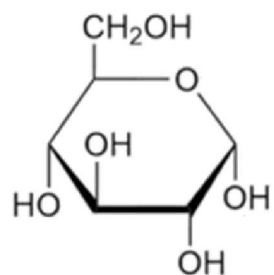




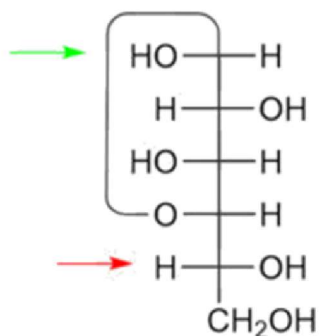


→ anomerní centrum

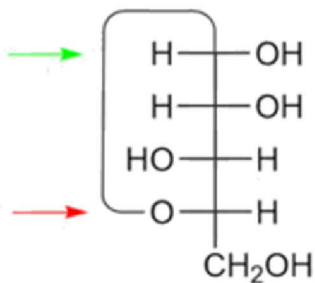
→ konfigurační atom



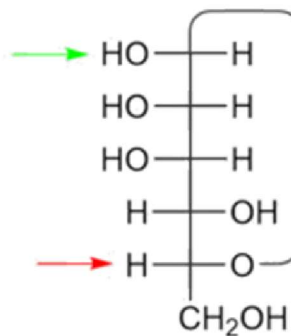
$\alpha$ -D-glukopyranosa



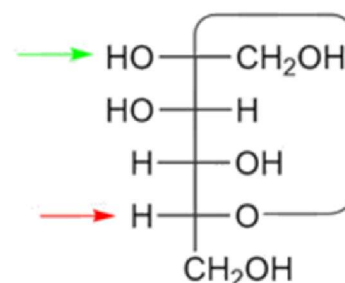
$\beta$ -D-galaktofuranosa




$\beta$ -L-arabinofuranosa



$\beta$ -D-mannopyranosa



$\beta$ -D-fruktofuranosa

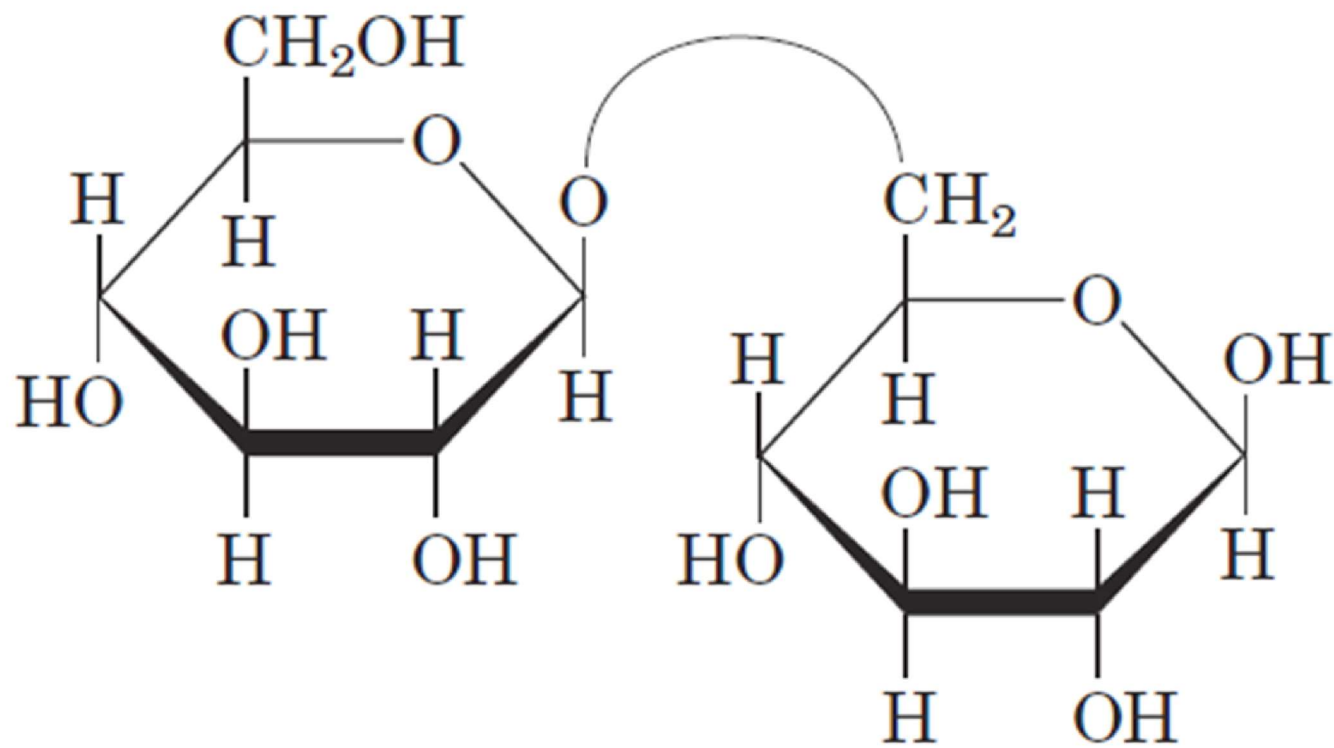


Nakreslete vzorec disacharidu  $\text{D-Glc}(\beta 1 \rightarrow 6)\text{D-Glc}$   
Je tento cukr redukující?

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Nakreslete vzorec disacharidu  $\text{D-Glc}(\beta 1 \rightarrow 6)\text{D-Glc}$   
Je tento cukr redukující?

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Tento cukr je redukující