

NBCM-010

Bioorganická chemie

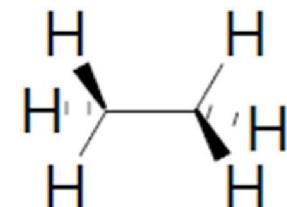
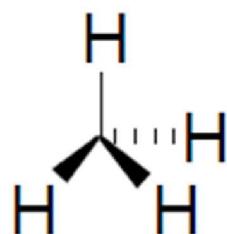
Cvičení – konformace CIP pravidla

Kateřina Hofbauerová

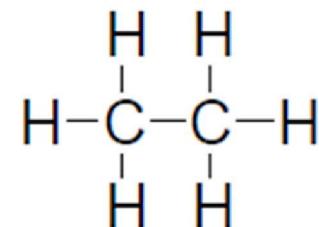
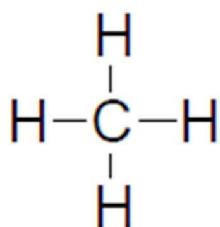


vzorce

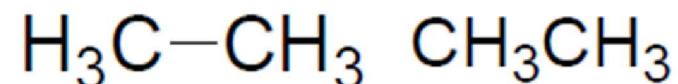
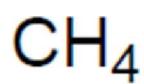
perspektivní



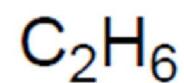
strukturní

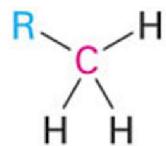


zjednodušené strukturní



souhrnné (sumární)

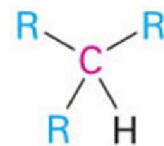




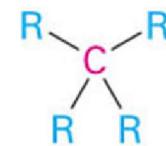
Primary carbon (1°)
is bonded to one
other carbon.



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



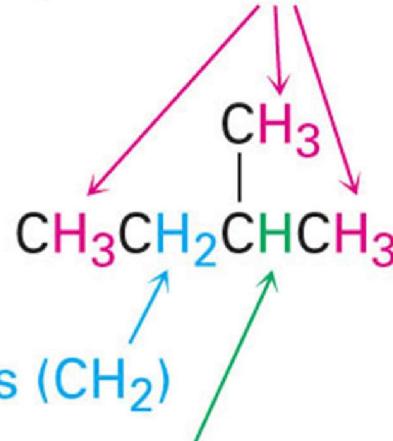
Tertiary carbon (3°)
is bonded to three
other carbons.



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

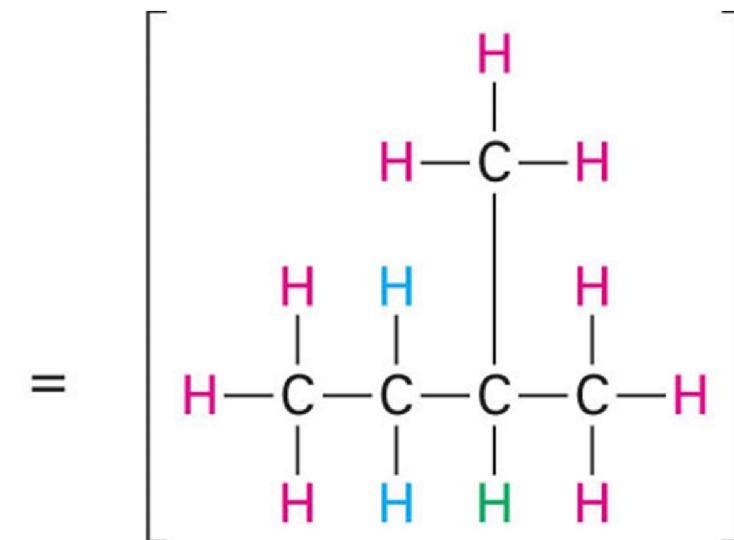
© 2007 Thomson Higher Education

Primary hydrogens (CH_3)



Secondary hydrogens (CH_2)

A tertiary hydrogen (CH)



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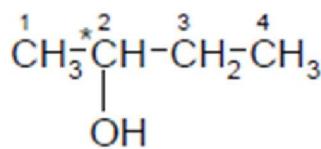
CIP pravidla

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

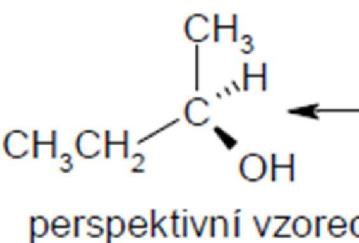
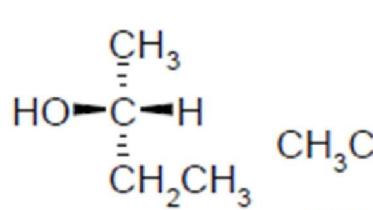
Pravidlo posloupnosti představuje způsob, jakým se určuje nadřazenost skupin, substituentů i ligandů kolem stereogenního centra. V prvním přiblížení posta je pořadí podle klesajících protonových hodnot atomů bezprostředně k nimu vázaných, např. Cl > S > F > O > N > C; podobně se pokračuje v dalším přiblížení, např. CH₂Cl > CH₂OH > > CH₂CH₃ > CH₃. Substituent může se přidat i 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 hydroxyskupinu náležet **1**, ethylu **2**, methylu **3** a vodíkovému atomu **4**.

Smysl chirality - 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 (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** píší kurzívou, umísťují se v závorkách před úplný název sloučeniny, odděleny ho. Se oddělují spojovníkem.

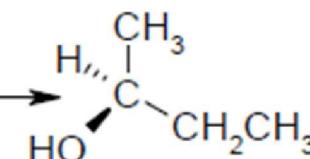
Ekvimolární směs pár enantiomerů (1:1) se nazývá racemát.



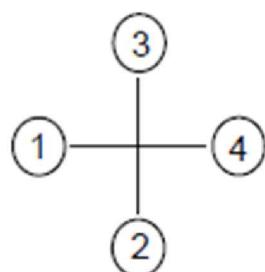
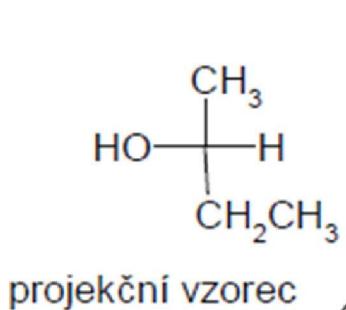
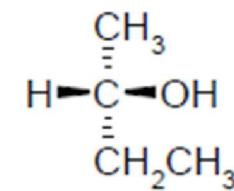
konstituční vzorec



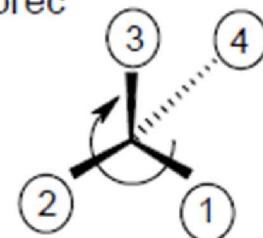
perspektivní vzorec



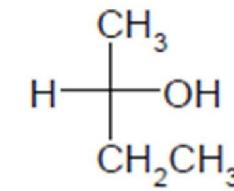
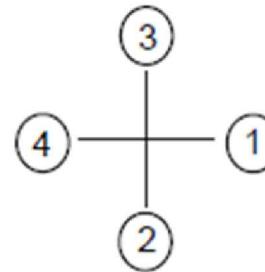
perspektivní vzorec



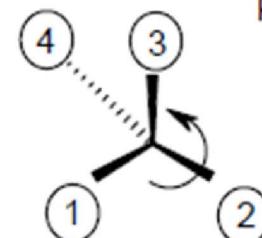
projekční vzorec



(R)-butan-2-ol
 $[\alpha]_D^{27} = -13,5$

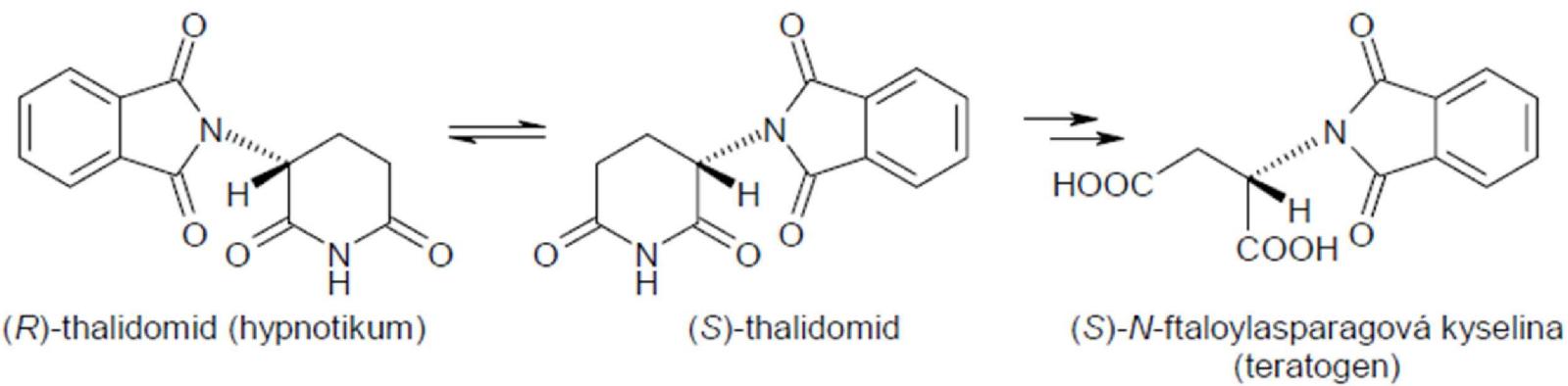
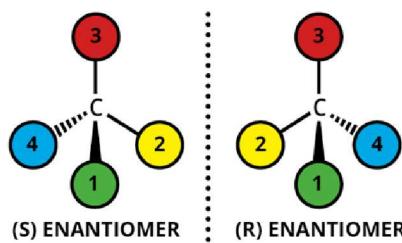


projekční vzorec



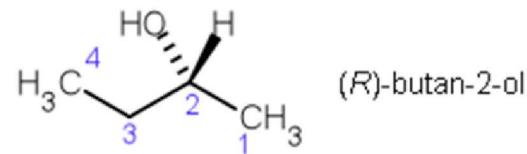
(S)-butan-2-ol
 $[\alpha]_D^{27} = +13,5$

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

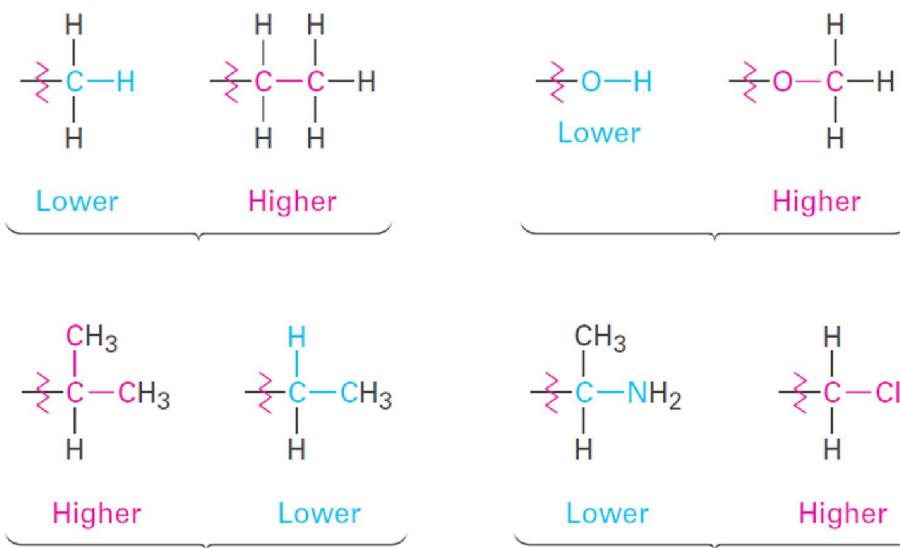


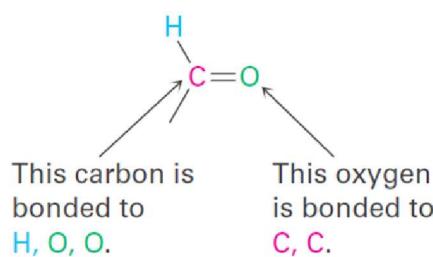
Postup převodu názvu na strukturu

Struktura	Název	Poznámka
	butan	Základ názvu
		Číslování
	butan-2-ol	
	(R)-butan-2-ol	Kompletní struktura

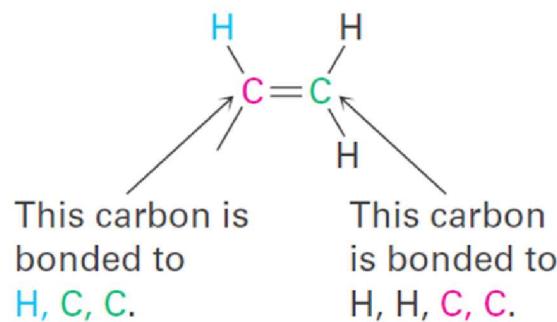
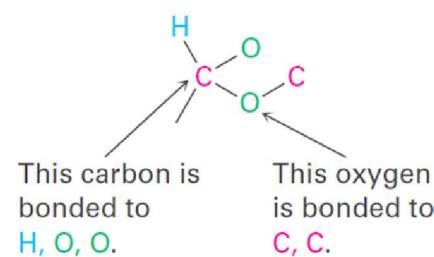
Substituent m se p i adí ísla v po adí klesající priority, tedy v po adí **1 > 2 > 3 > 4**, kde symbol > znamená, že je nad azen, ve smyslu pravidla posloupnosti.
V p ípad butan-2-olu tak bude hydroxyskupin náležet **1**, ethylu **2**, methylu **3** a vodíkovému atomu **4**.

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

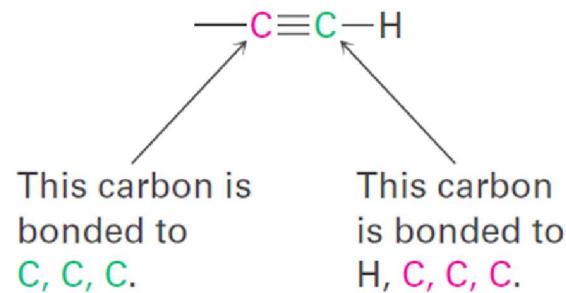
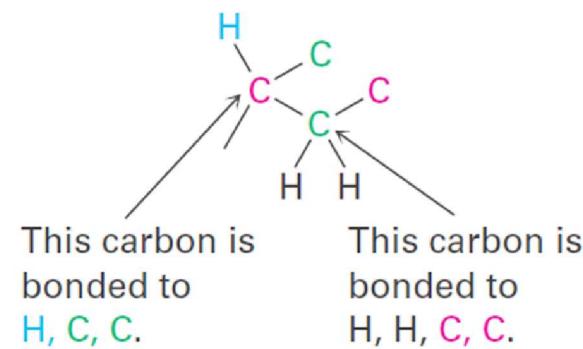




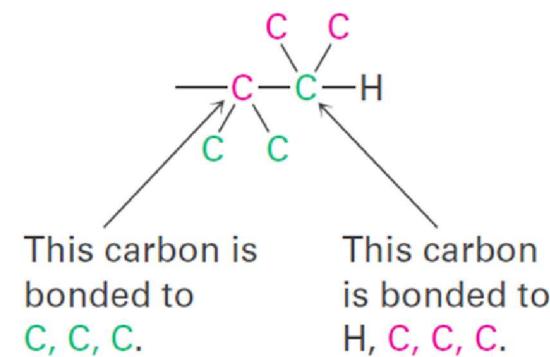
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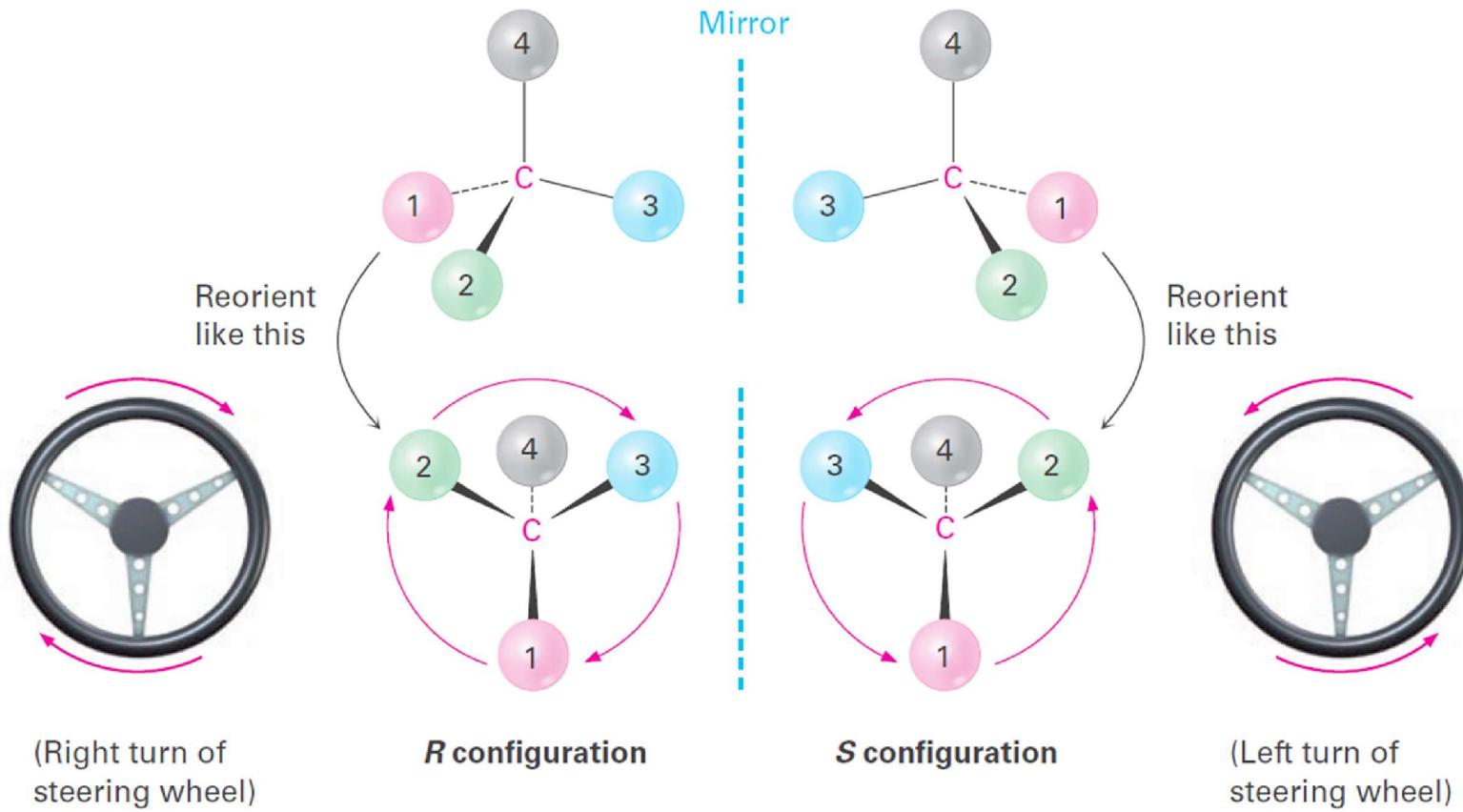


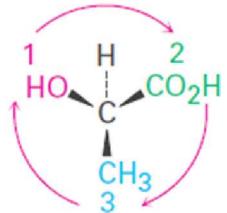
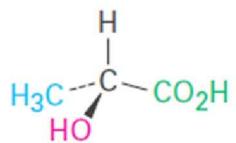
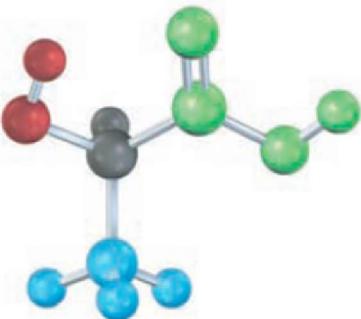
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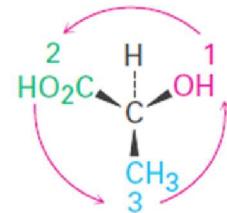
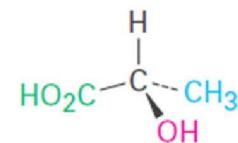
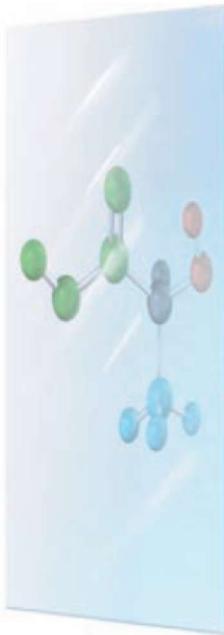
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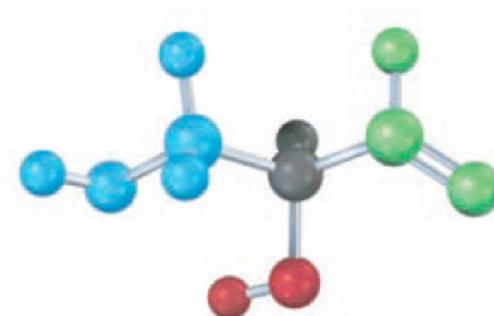
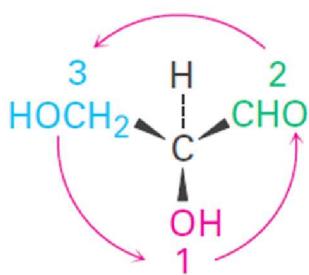
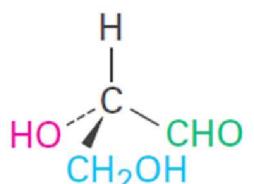




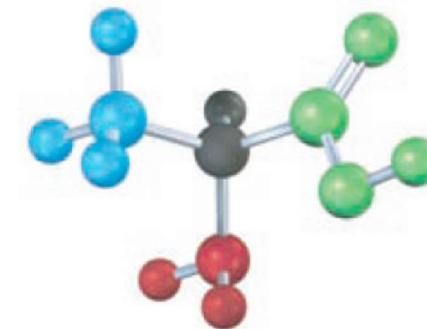
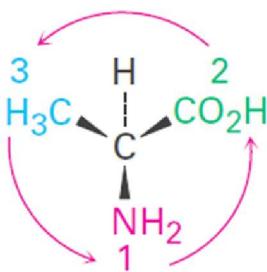
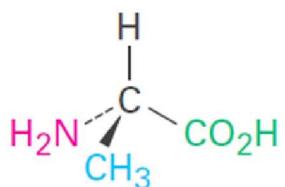
R configuration
 (R) - $(-)$ -lactic acid



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

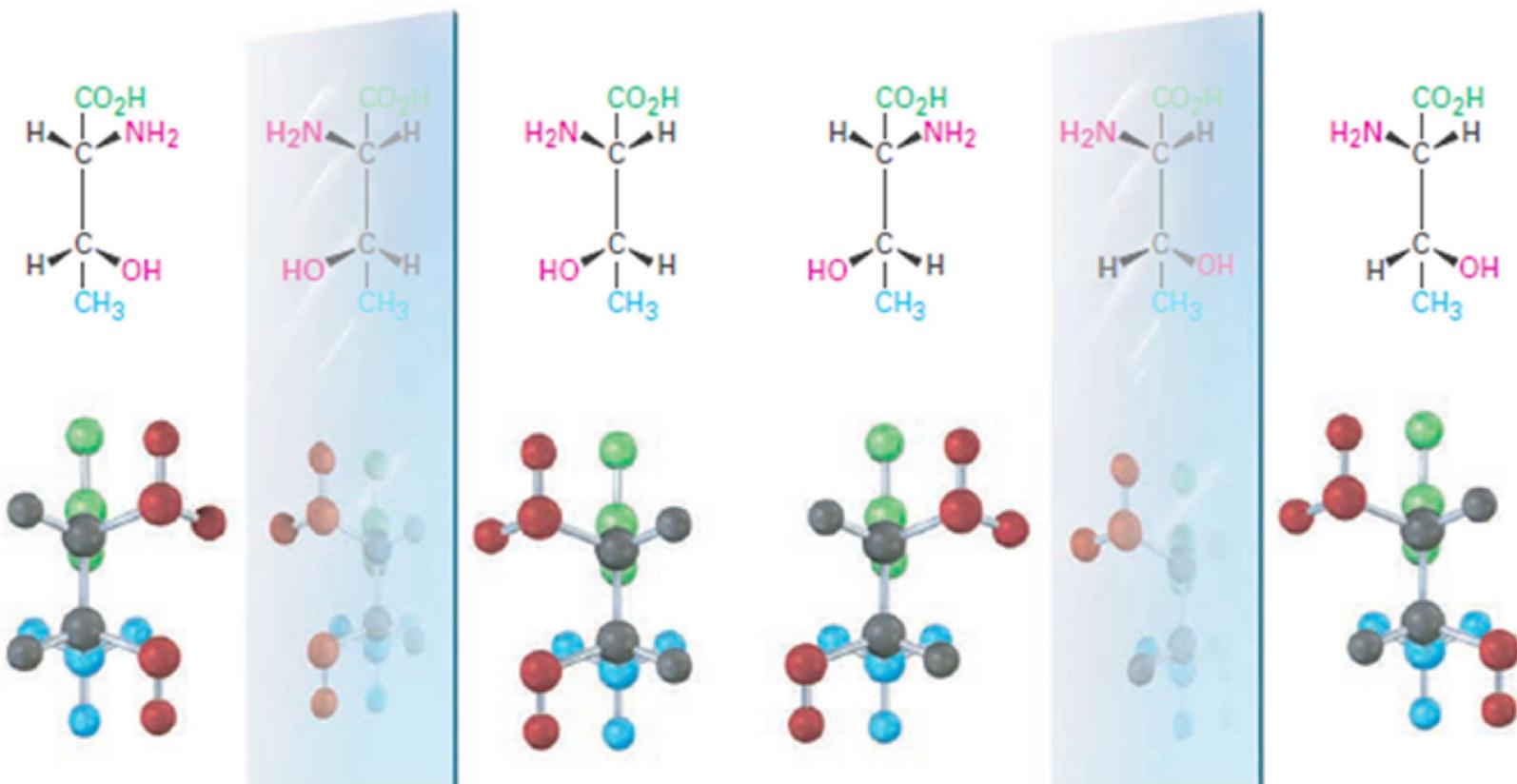


(*S*)-Glyceraldehyde
[(*S*)-(-)-2,3-Dihydroxypropanal]
 $[\alpha]_D = -8.7$



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

Určete absolutní konfiguraci



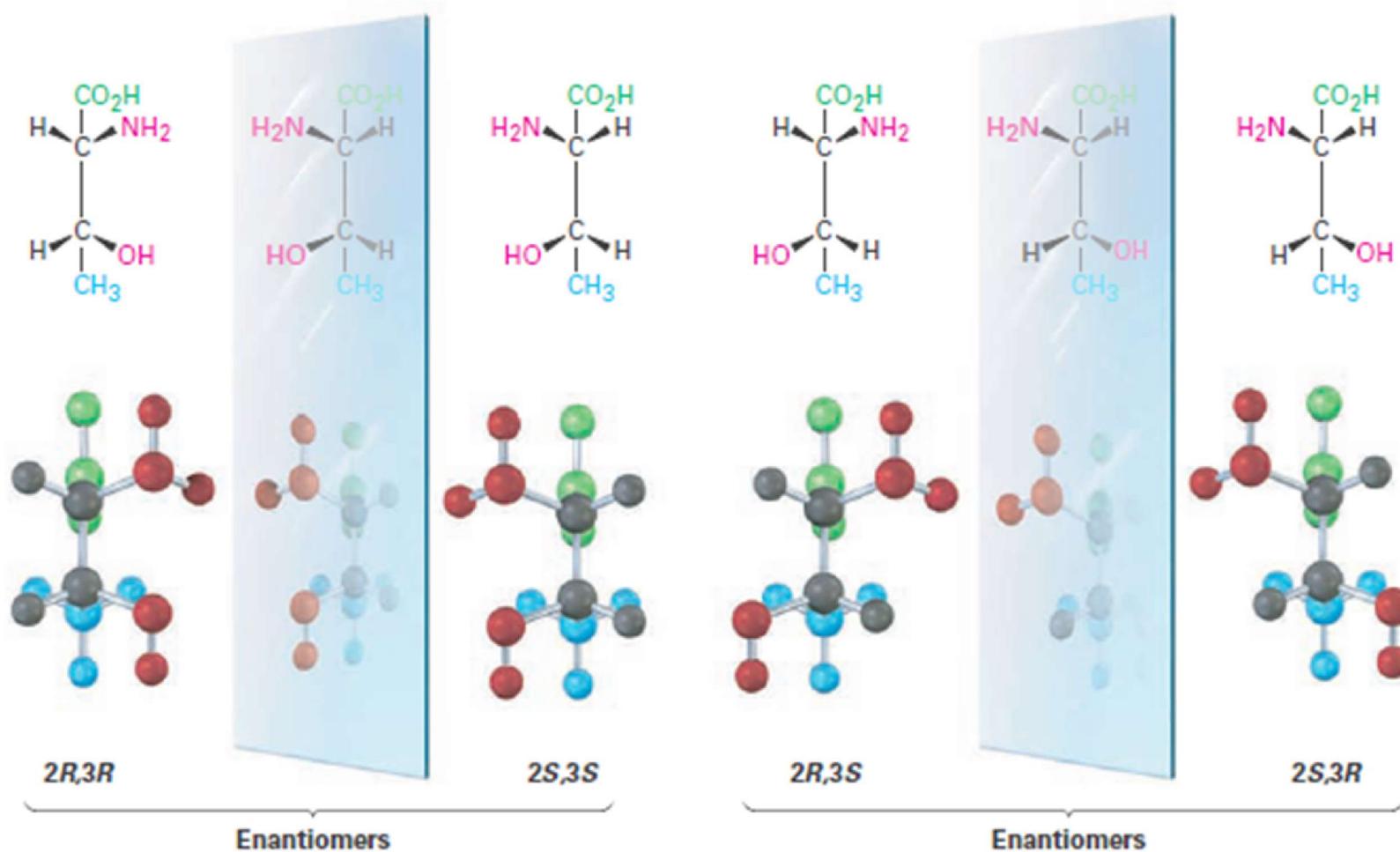


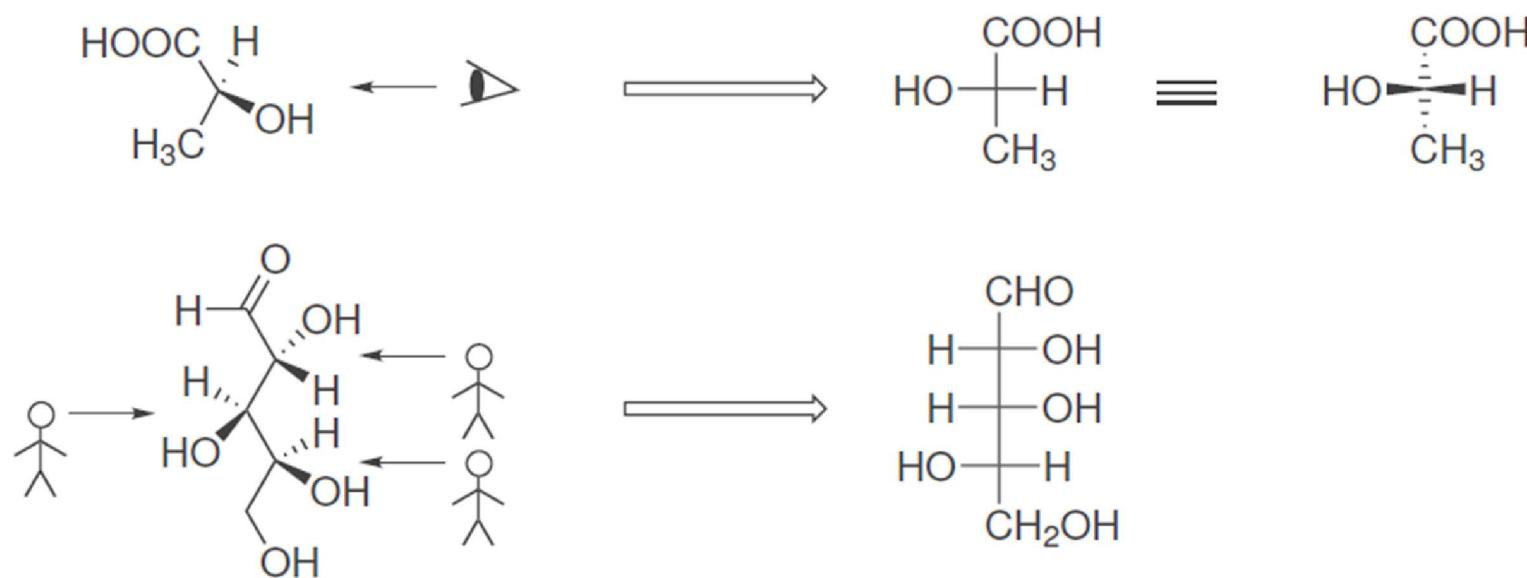
FIGURE 5.10 The four stereoisomers of 2-amino-3-hydroxybutanoic acid.

2-amino-3-hydroxybutanová kyselina

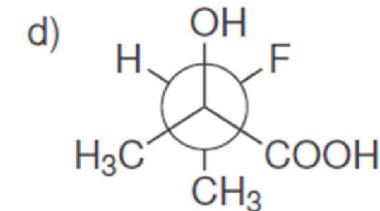
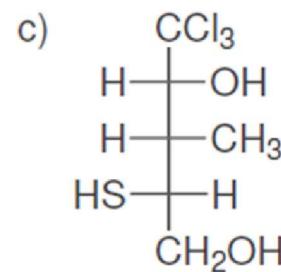
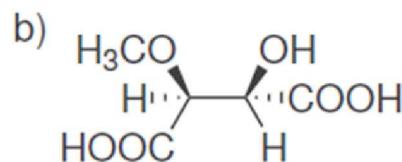
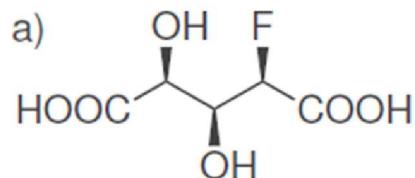
Aminokyselina threonin - (2S,3R)-2-amino-3-hydroxybutanová kyselina

Fischerova projekce

Nejástejněji používána pro znázornění prostorového uspořádání sacharidů a podobných derivátů.



Pojmenujte sloučeniny, určete absolutní konfiguraci a překleslete z nebo do Fisherovy projekce

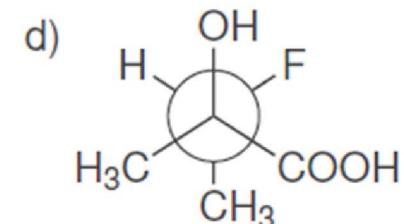
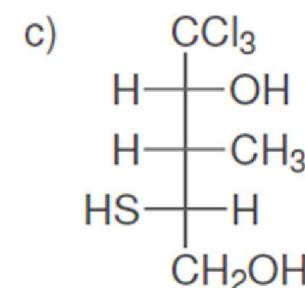
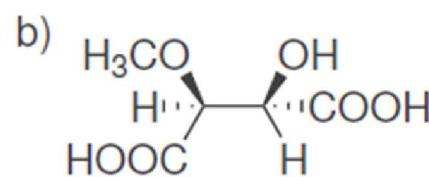
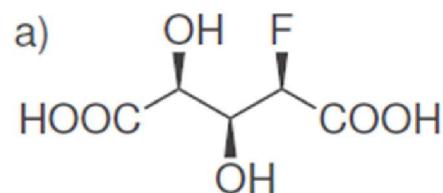


klínkové
zobrazení

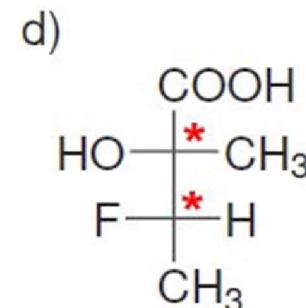
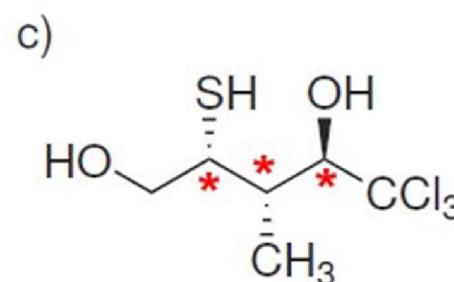
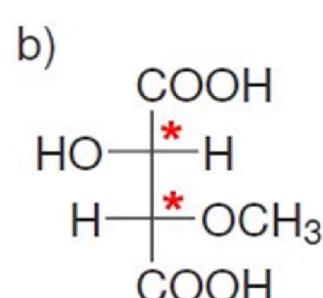
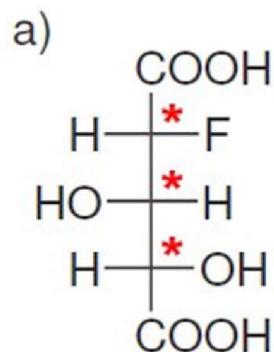
Fisherova
projekce

Newmanova
projekce

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

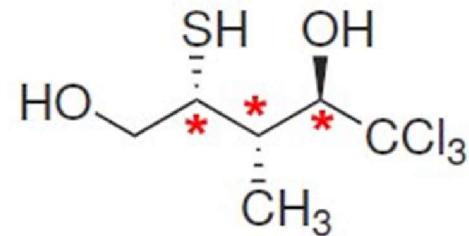


Zobrazení v projekci a označení stereogenních center

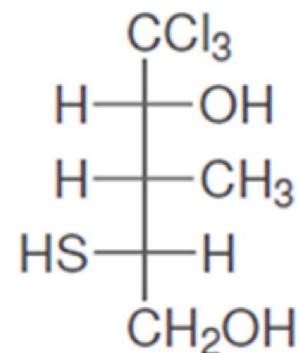
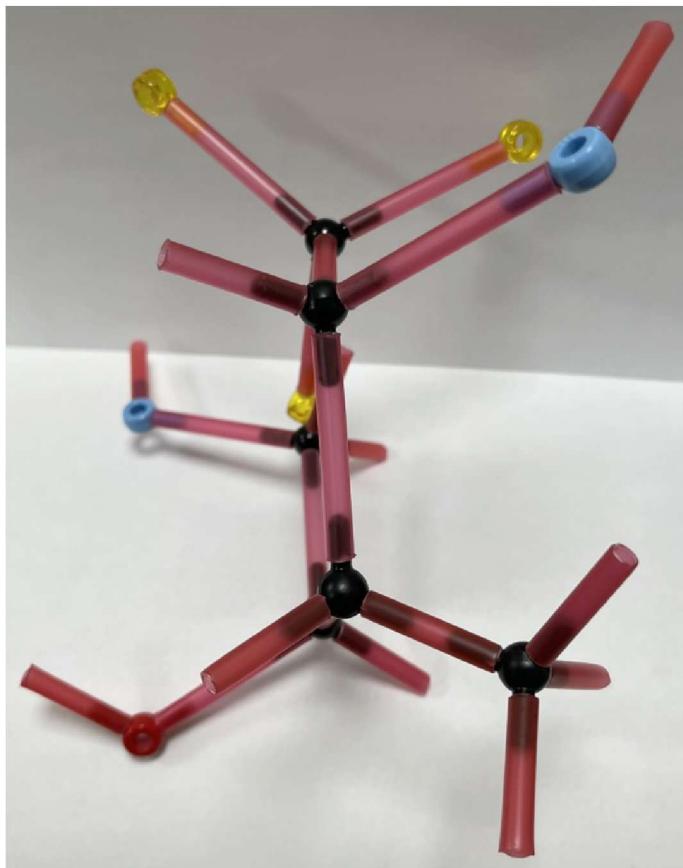


Pořadí dle ležitosti podle protonových čísel
 Cl 17 > S 16 > F 9 > O 8 > N 7 > C 6 > H 1

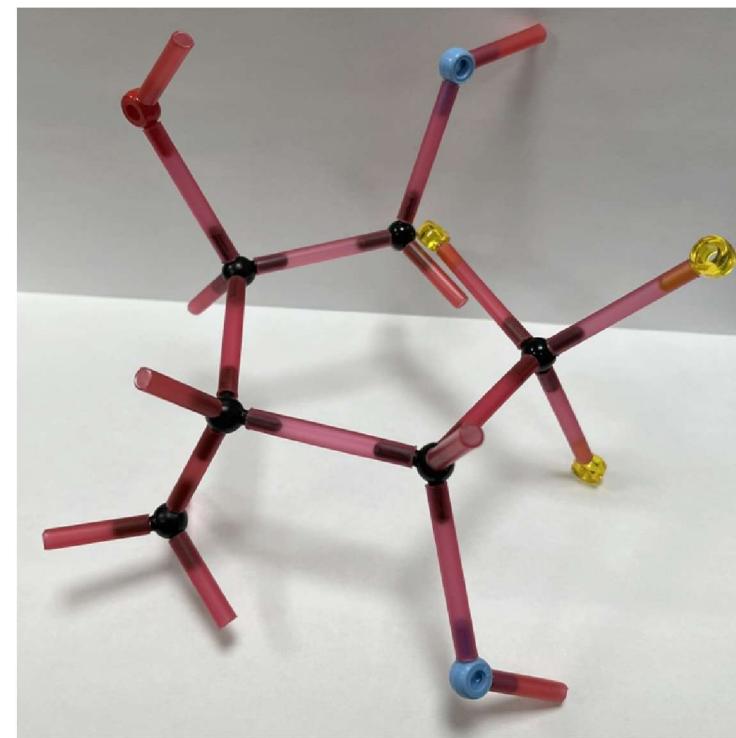
c)



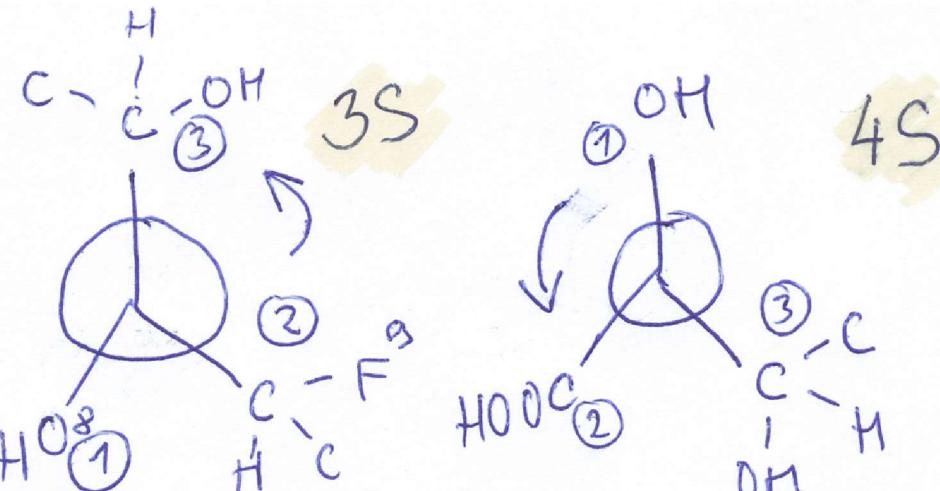
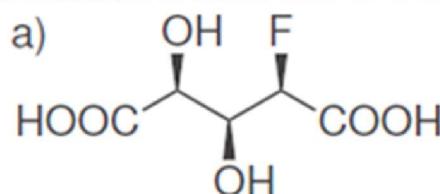
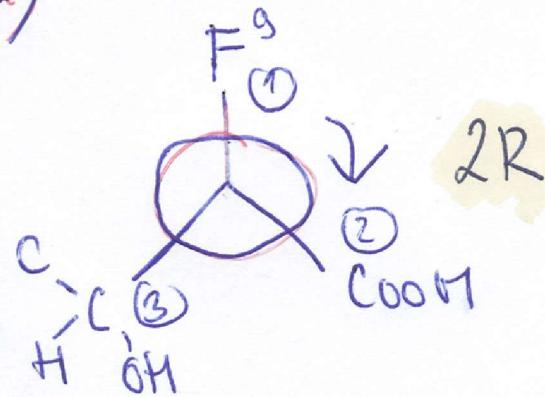
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Fisherova projekce

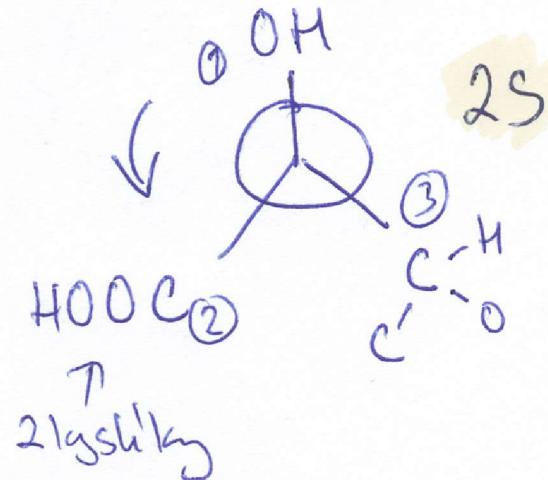
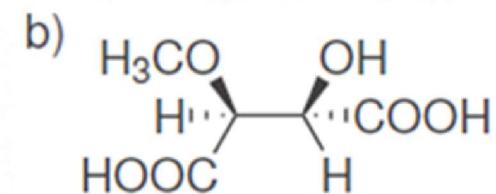


a)

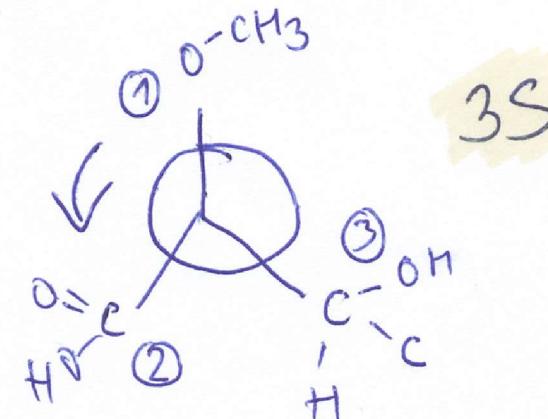


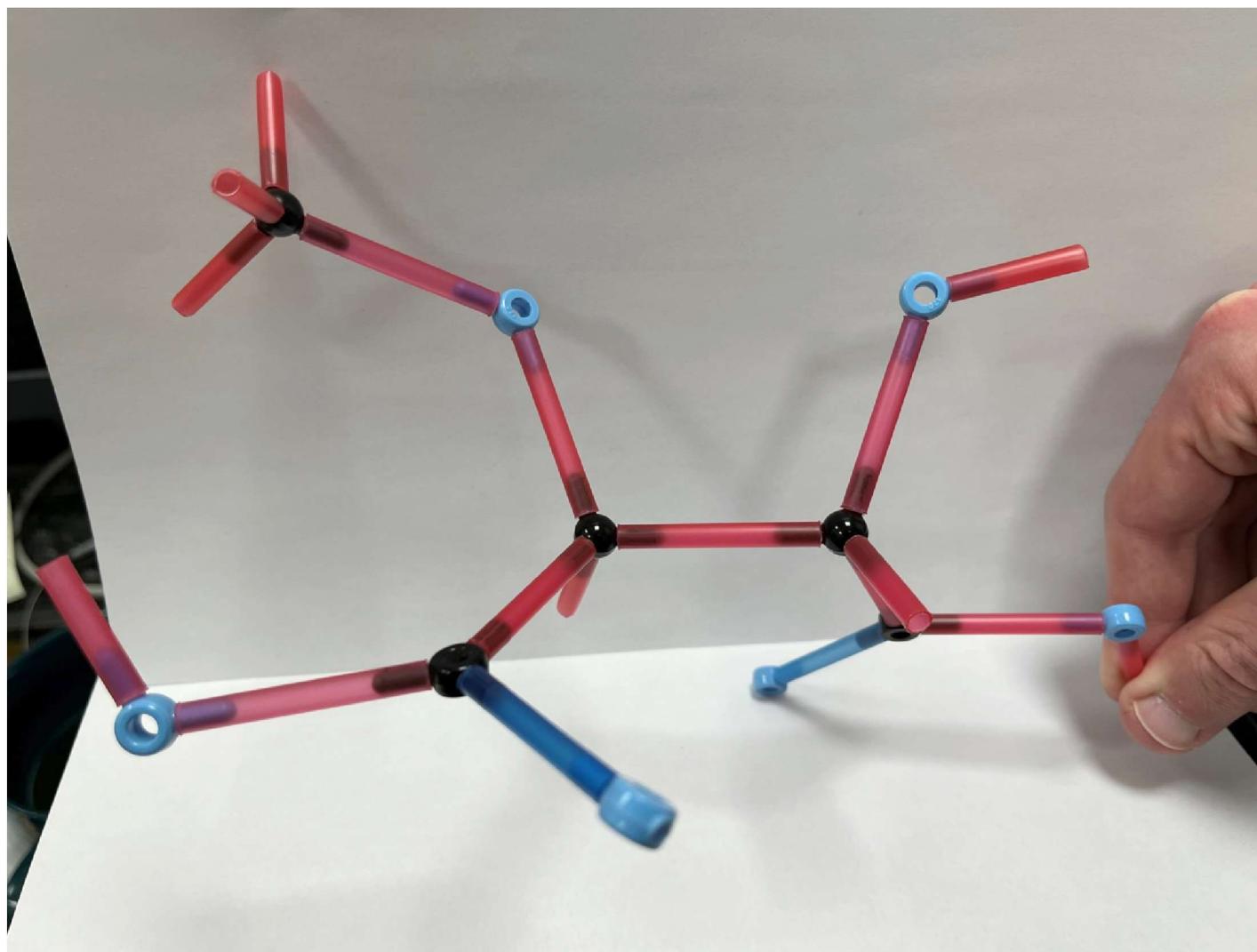
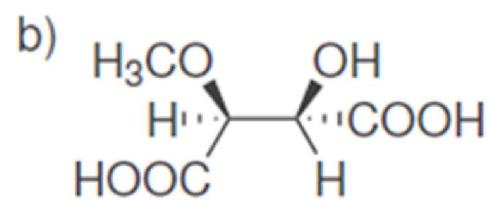
vodík dozadu

b) pro pozici 2 v původním zobrazení
ukážit molekulu; H1 směřuje pod plánem

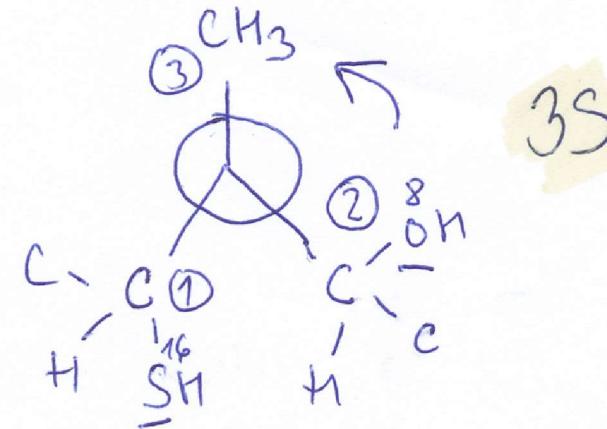
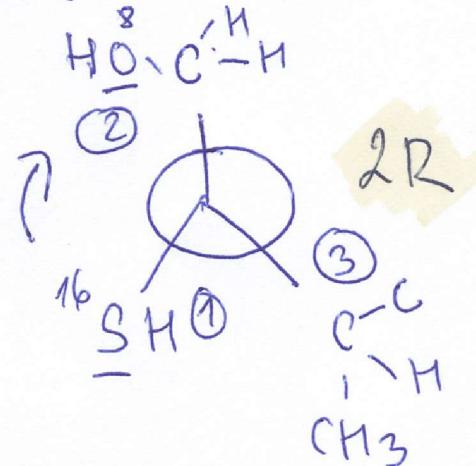


21gšíky

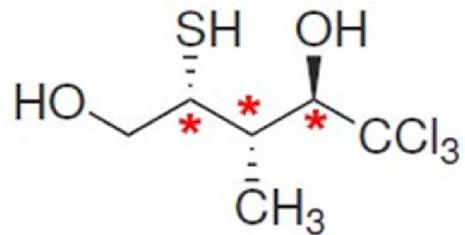




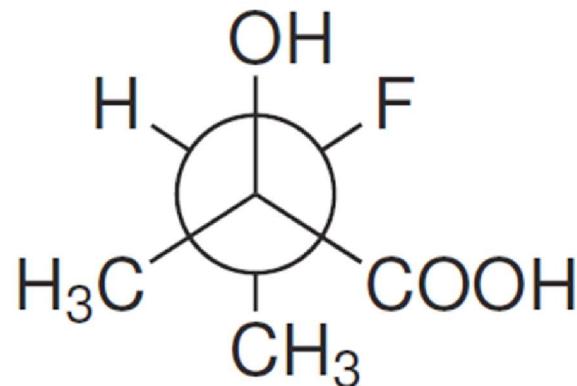
c) pro pozici 2 a 3 vstříln molekuly; H směřuje pod pladem



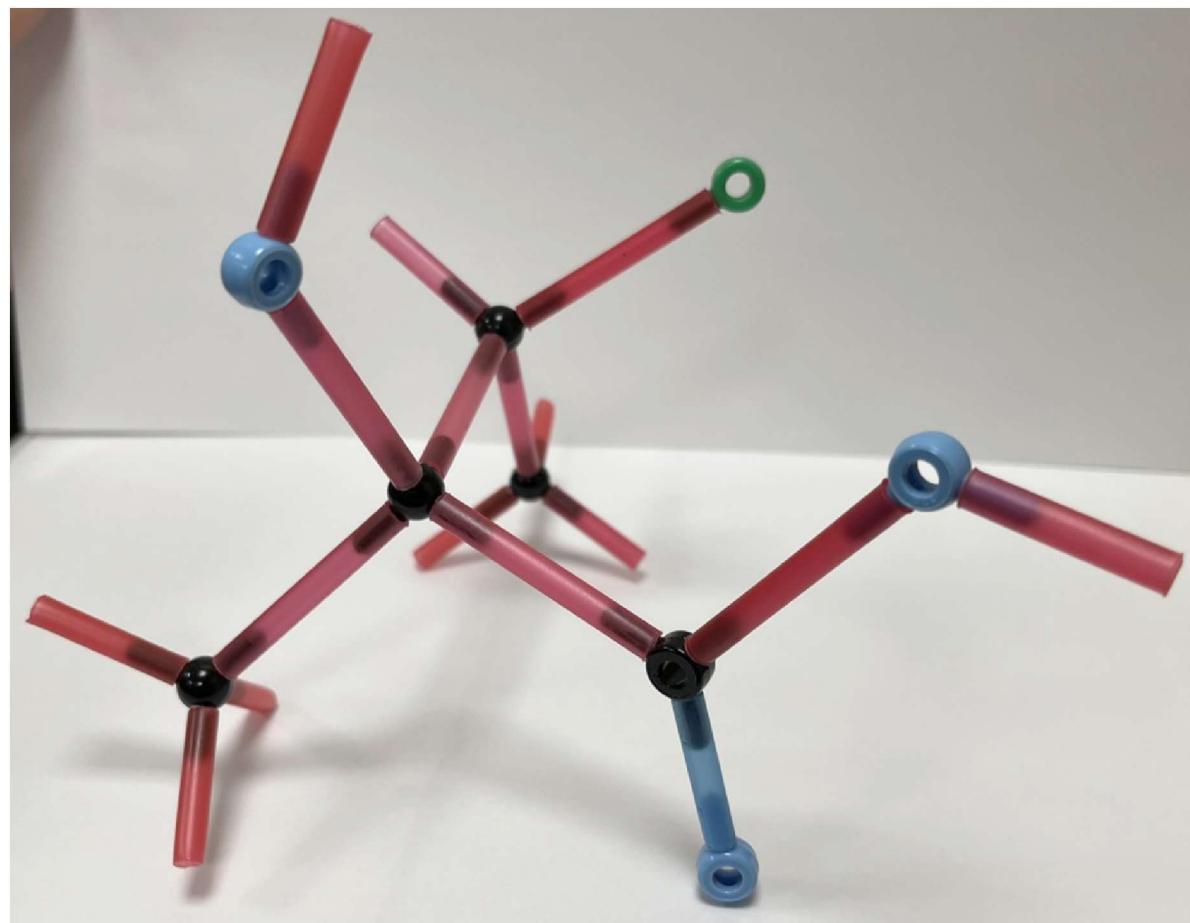
c)

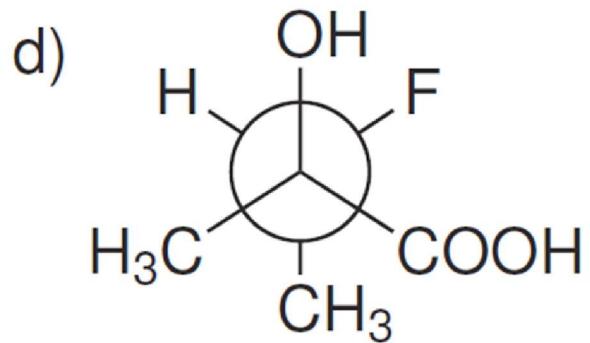


d)

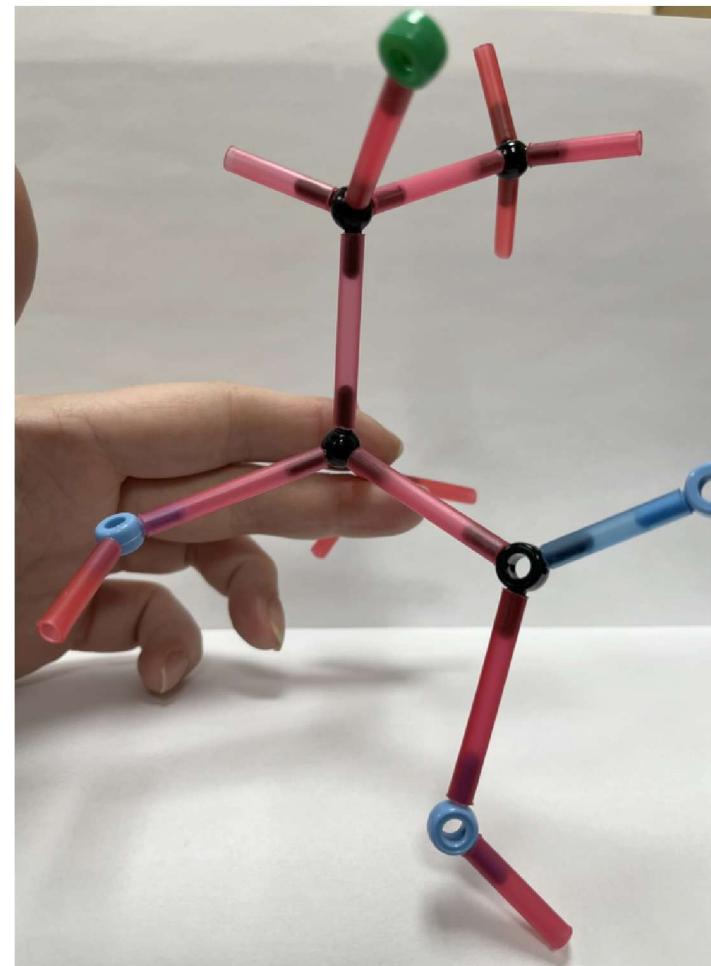
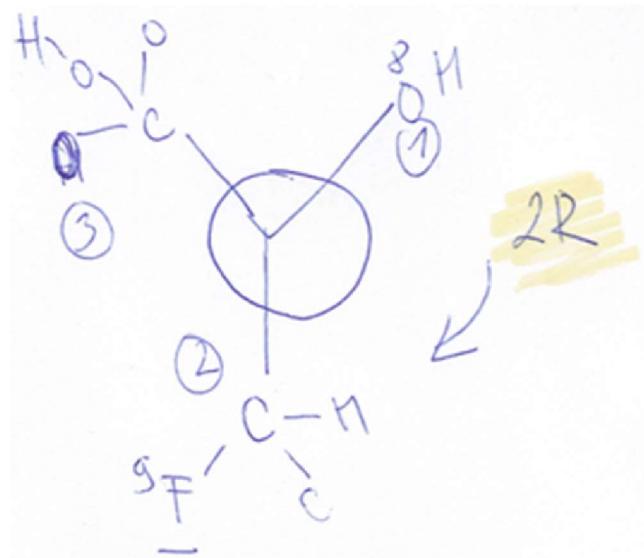


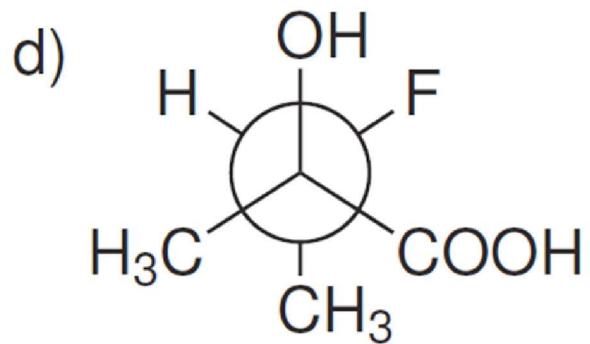
Místo vodík jsou na fotografii
kratší vazby, kyslík je modré,
fluor zelené, dvojná vazba modré



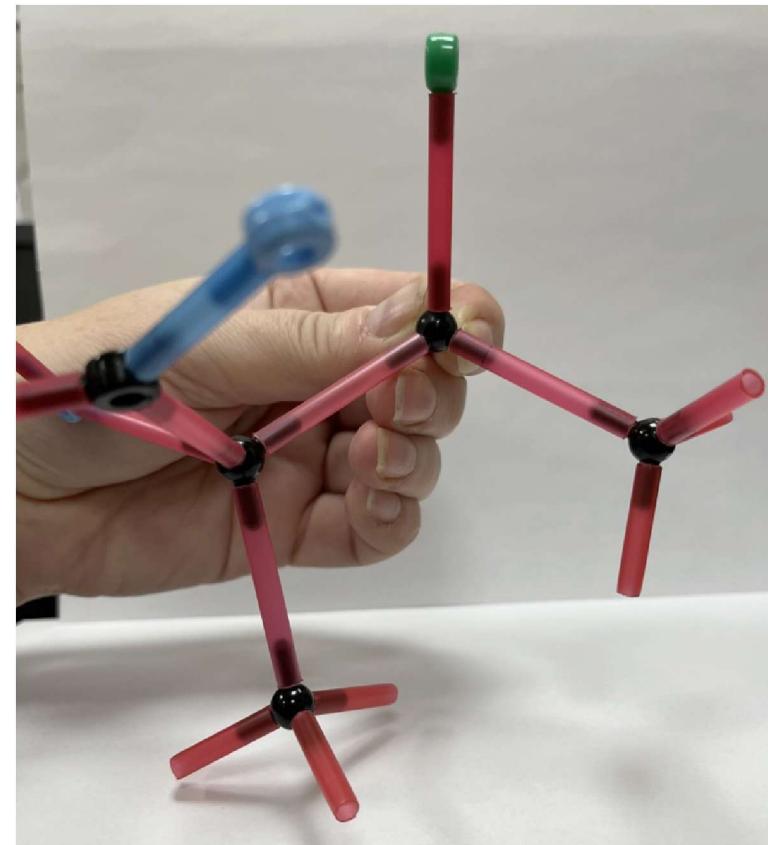
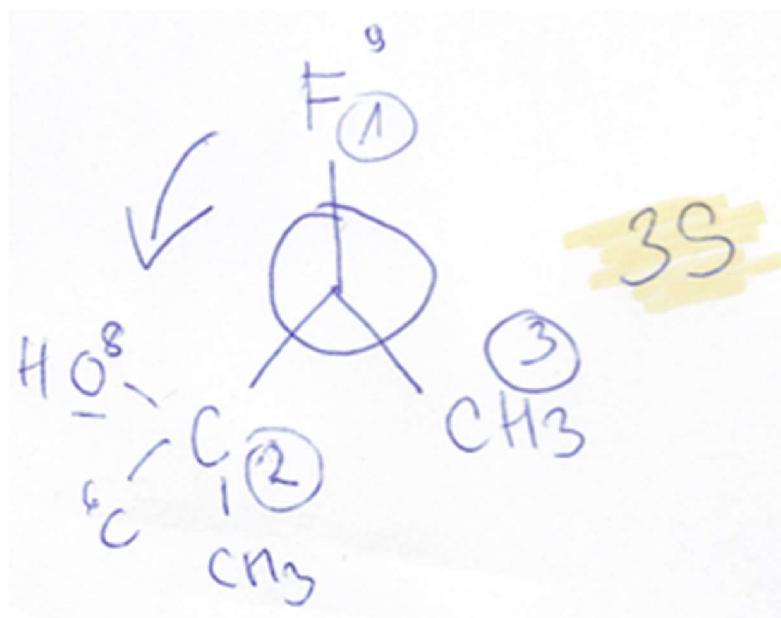


Místo vodík jsou na fotografii kratší vazby, kyslík je modré, fluor zelené, dvojná vazba modré

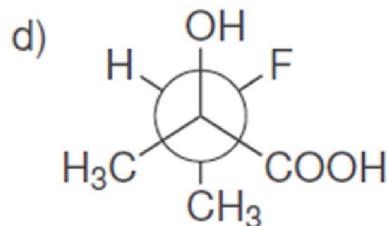
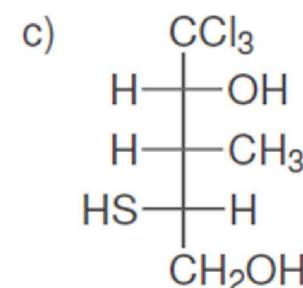
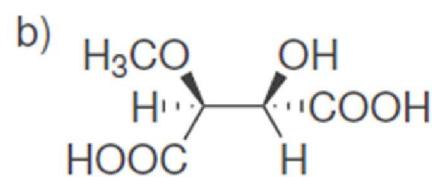
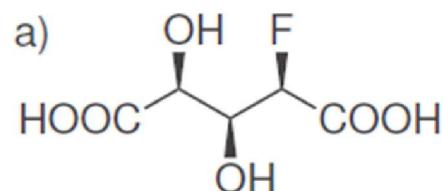




Místo vodík jsou na fotografii
kratší vazby, kyslík je modré, e,
fluor zelené, dvojná vazba modré



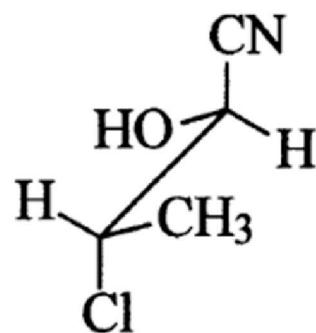
Pojmenujte sloučeniny, určete absolutní konfiguraci a překleslete z nebo do Fischerovy projekce



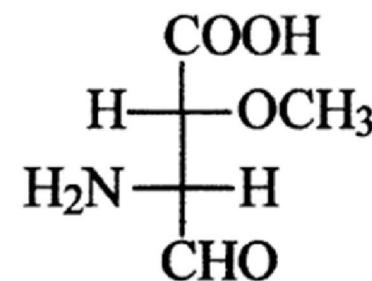
- (a) (2R,3S,4S)-2-fluor-3,4-dihydroxypentan-1,5-diová kyselina
- (b) (2S,3S)-2-hydroxy-3-methoxybutan-1,4-butandiová kyselina
- (c) (2R,3S,4R)-5,5,5-trichlor-3-methyl-2-sulfanylpentan-1,4-diol
- (d) (2R,3S)-3-fluor-2-hydroxy-2-methylbutanová kyselina

Určete absolutní konfiguraci sloučenin

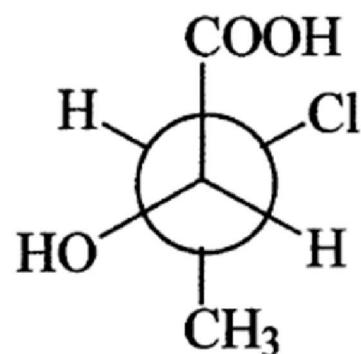
a)



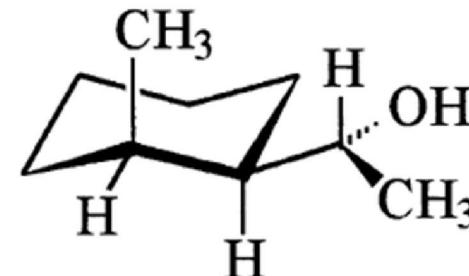
b)



c)



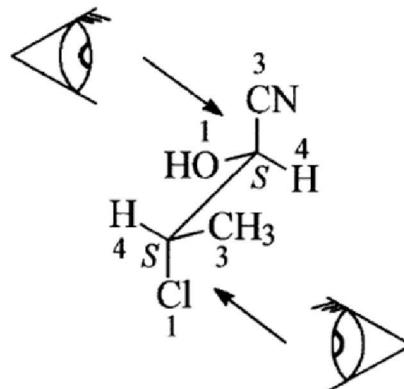
d)



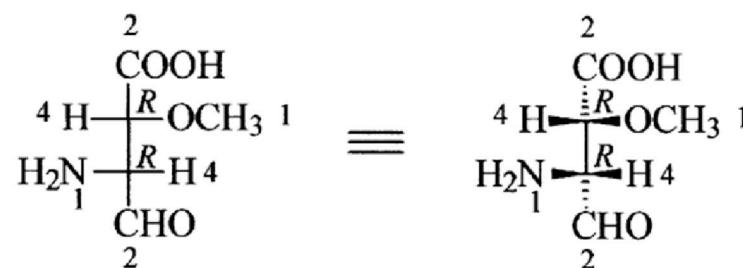
Newmanova projekce

Určete absolutní konfiguraci sloučenin

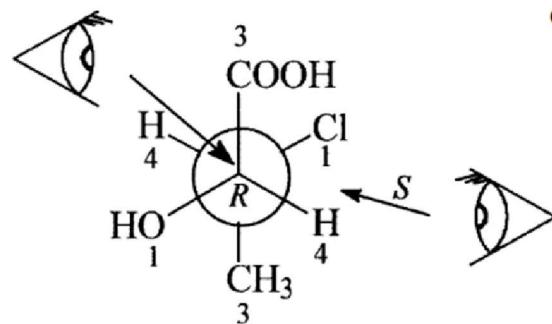
a)



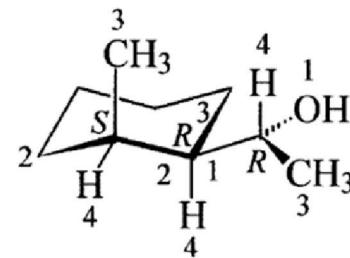
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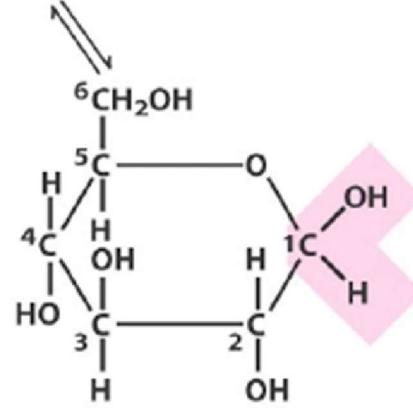
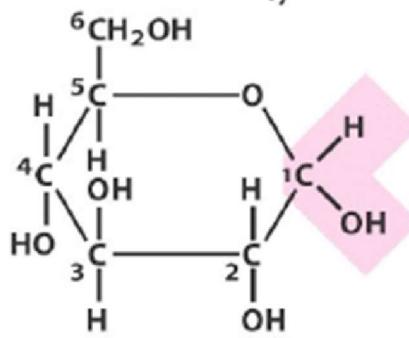
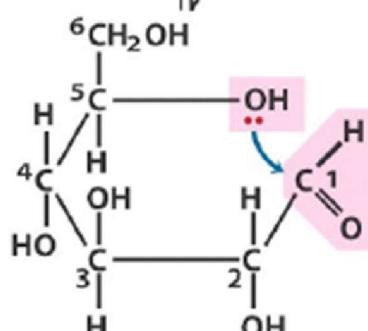
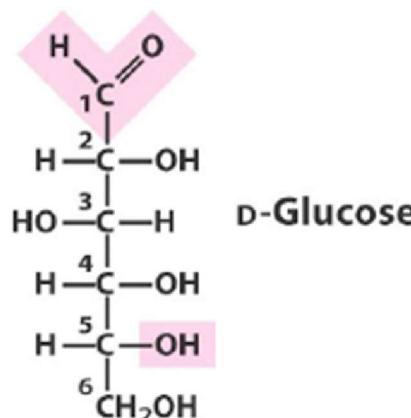


c)



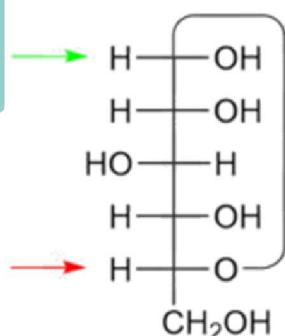
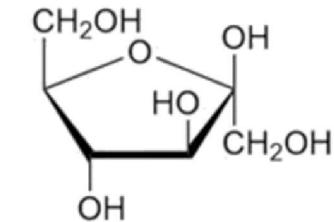
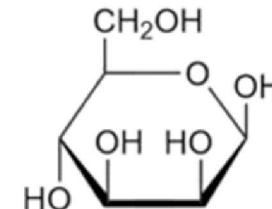
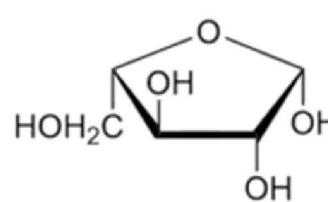
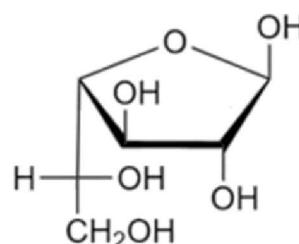
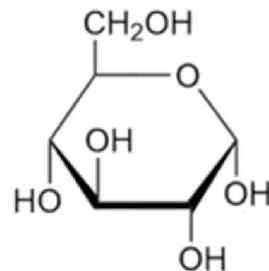
d)



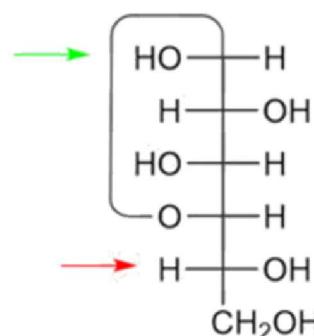




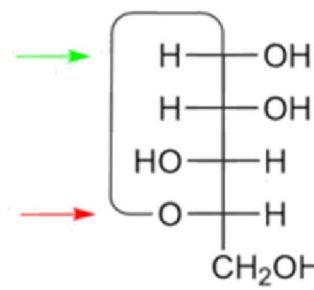
→ anomerní centrum
→ konfigurační atom



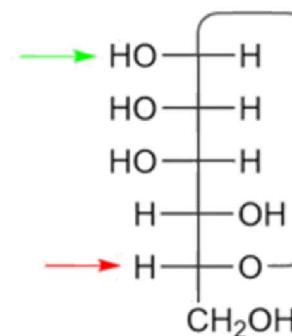
α -D-glukopyranosa



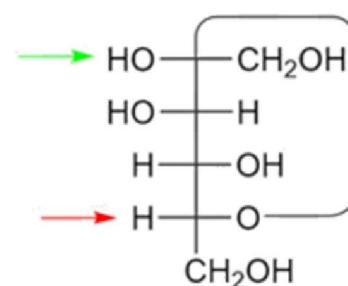
β -D-galaktofuranosa



β -L-arabinofuranosa



β -D-mannopyranosa

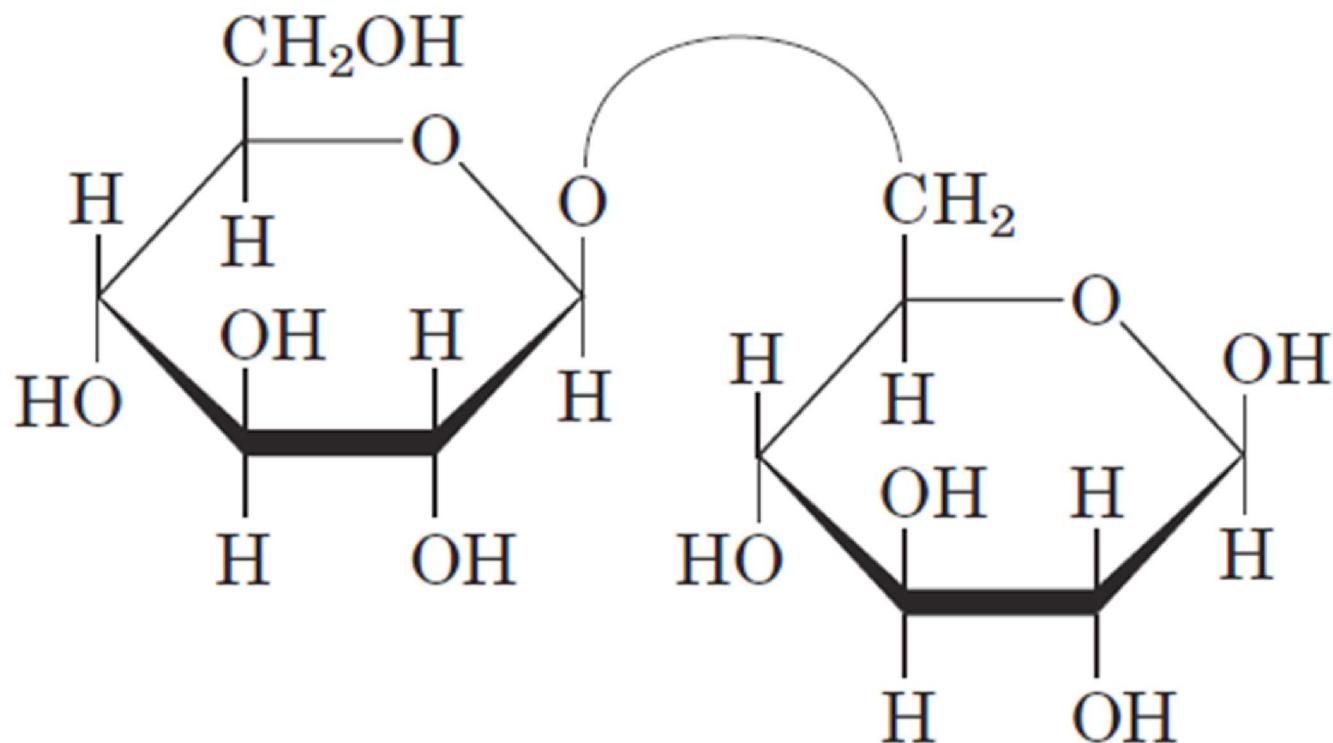


β -D-fruktofuranosa



Nakreslete vzorec disacharidu D-Glc(β 1→6)D-Glc
Je tento cukr redukující?

Nakreslete vzorec disacharidu D-Glc(β 1 \rightarrow 6)D-Glc
Je tento cukr redukující?



Tento cukr je redukující