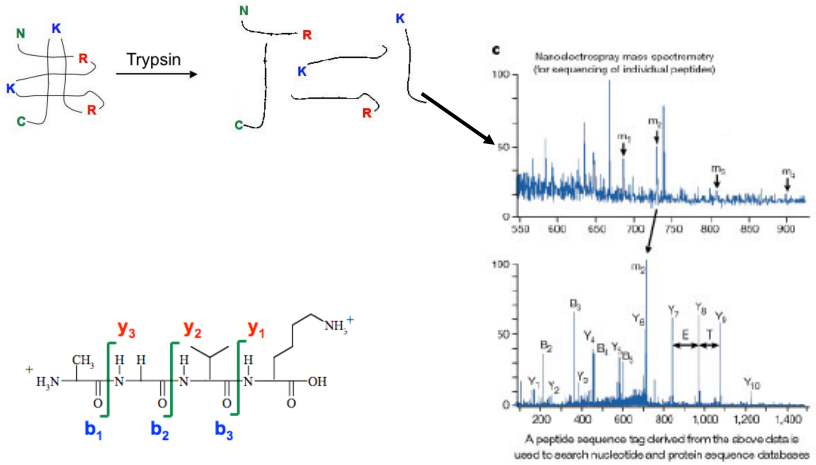
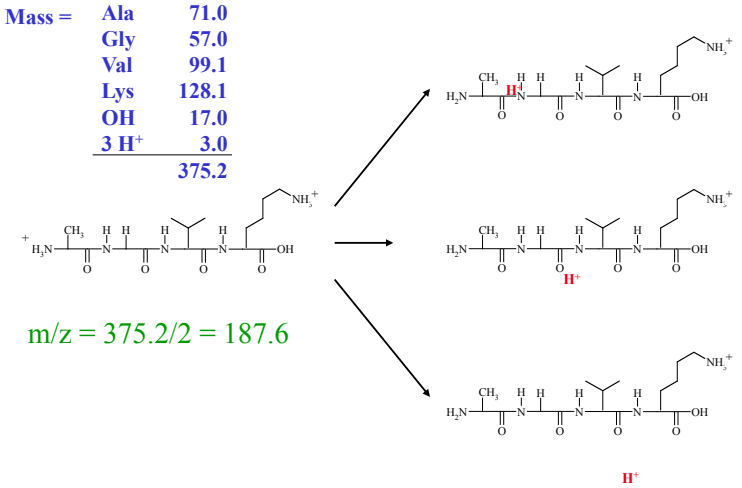
MS/MS Sequencing



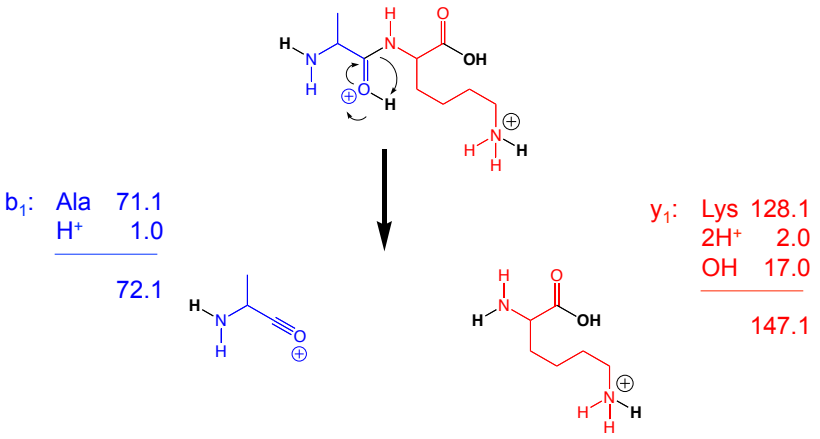
Properties of the Twenty

Amino Acid	Abbreviations	Residue Mass (Da)	Side Chain pK_a	$\Delta\Delta G^\circ_{transfer}$ (kcal/mol)
Alanine	Ala, A	71.09	-	-0.87
Arginine	Arg, R	156.19	**12**	15.93
Asparagine	Asn, N	114.11	-	5.22
Aspartic Acid	Asp, D	115.09	**4**	9.71
Cysteine	Cys, C	103.15	**8**	-0.34
Glutamine	Gln, Q	128.14	-	6.51
Glutamic Acid	Glu, E	129.12	**4**	7.78
Glycine	Gly, G	57.05	-	0.00
Histidine	His, H	137.14	**7**	5.63
Isoleucine	Ile, I	113.16	-	-4.00
Leucine	Leu, L	113.16	-	-4.00
Lysine	Lys, K	128.17	**10**	6.52
Methionine	Met, M	131.19	-	-1.42
Phenylalanine	Phe, F	147.18	-	-2.05
Proline	Pro, P	97.12	-	<0
Serine	Ser, S	87.08	-	4.36
Threonine	Thr, T	101.11	-	3.53
Tryptophan	Trp, W	186.21	-	-1.40
Tyrosine	Tyr, Y	163.18	**10**	1.09
Valine	Val, V	99.14	-	-3.11

Migration of N-terminal Proton

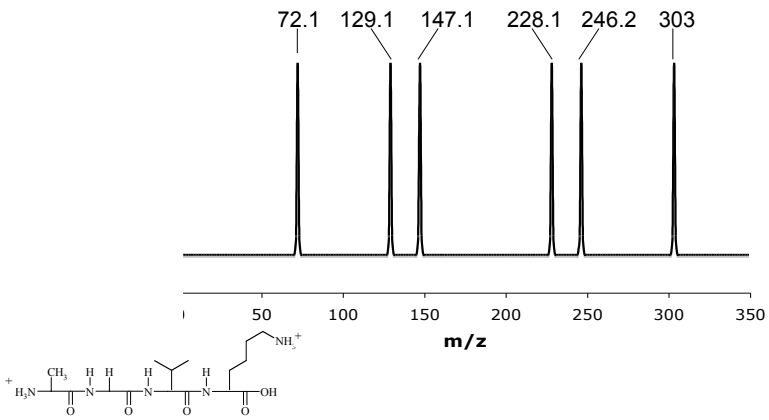


Collisionally Induced Dissociation

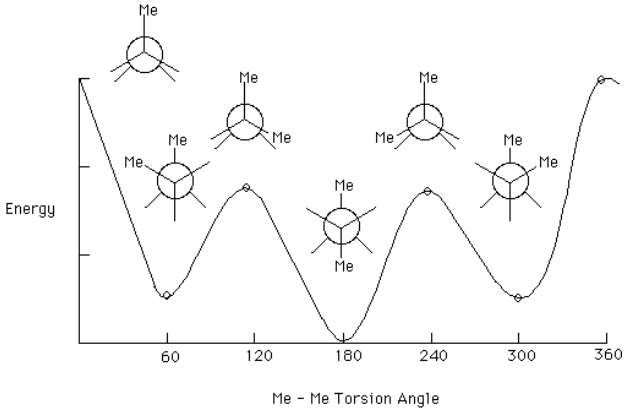


Fragment Spectrum of AGVK

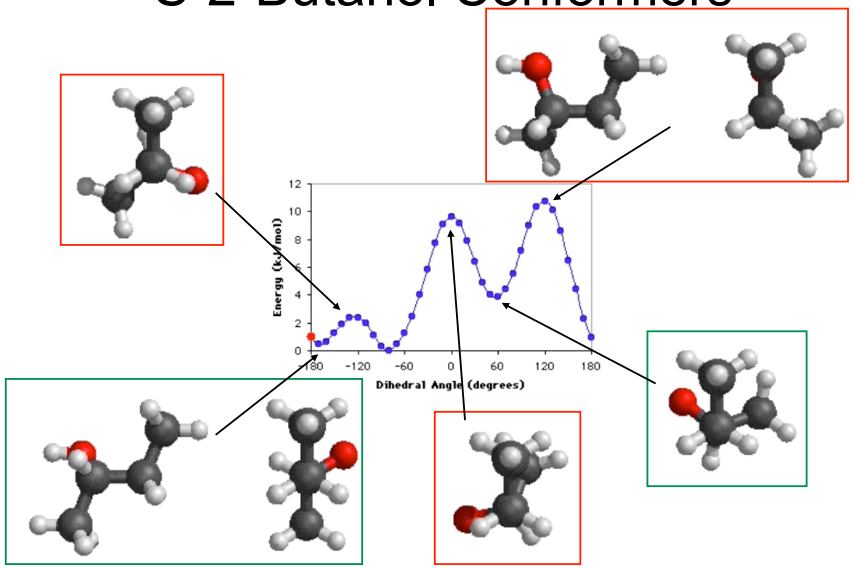
m/z = 375.2/2 = 187.6



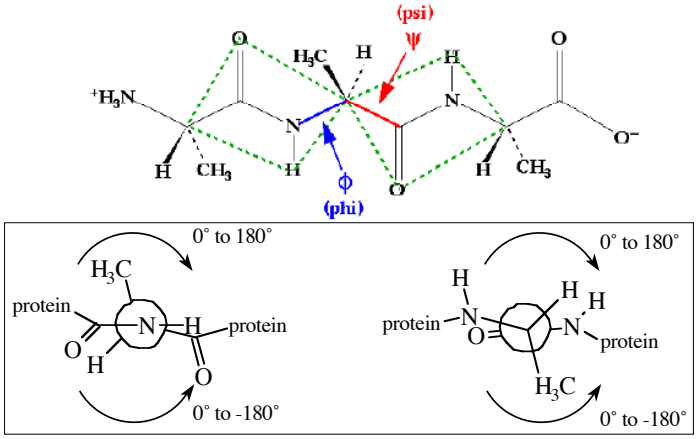
Butane Conformers



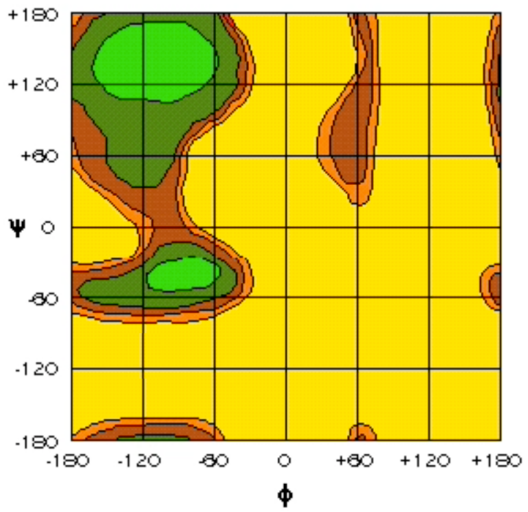
S-2-Butanol Conformers

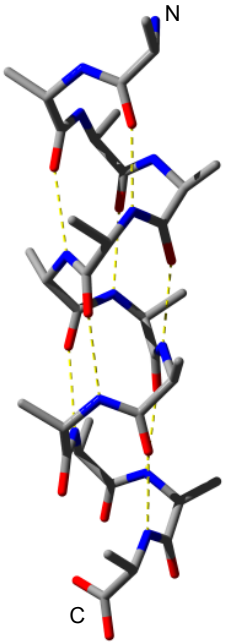


Phi (φ) and Psi (ψ) Dihedrals



Ramachandran plot





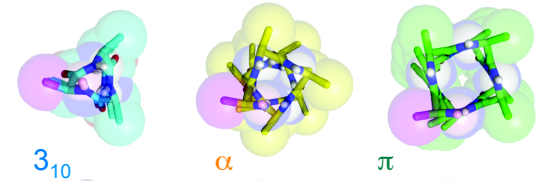
α-Helix Statistics

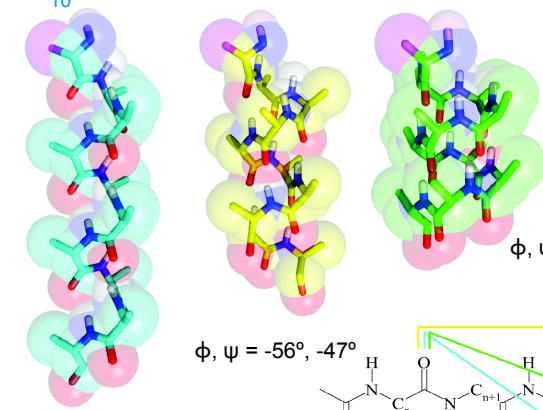
Right-handed twist

ϕ, ψ = -47˚, -57˚
3.6 residues/turn

Rise/AA along axis = 1.5 Å
Rise/turn along axis = 5.4 Å

Helix diameter = 4.6 Å



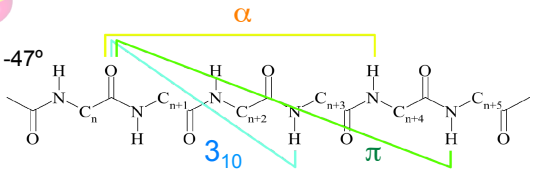


Three Possible
Right-handed
Helices

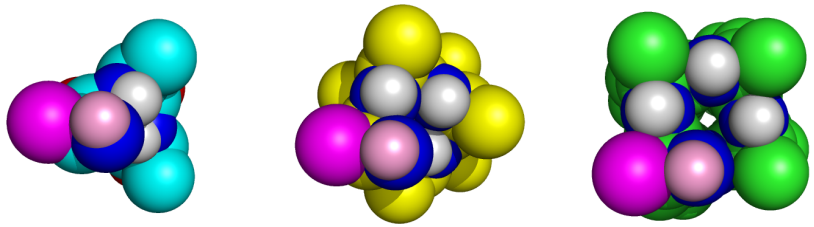
ϕ, ψ = -59°, -70°

ϕ, ψ = -56°, -47°

ϕ, ψ = -74°, -4°



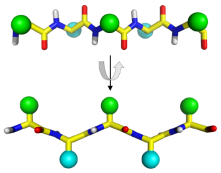
Three Helices



3_{10} α π

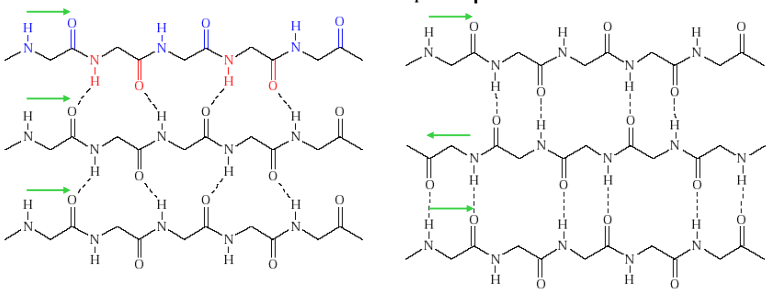
Beta Strands

$\varphi \approx -120^\circ$ to -140°, $\psi = 110^\circ$ to 130°

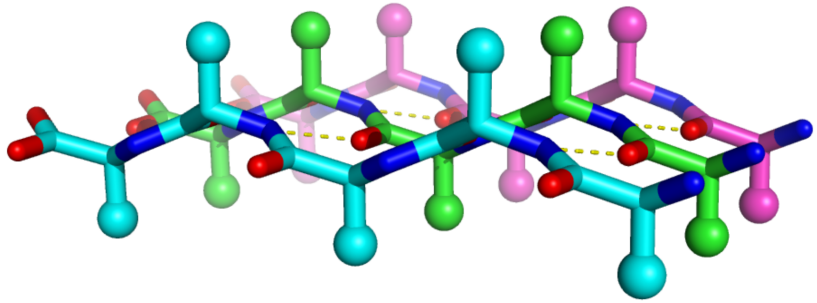


Parallel β–Sheet

Antiparallel β-Sheet



Beta Pleated Sheet



Beta (Reverse) Turn

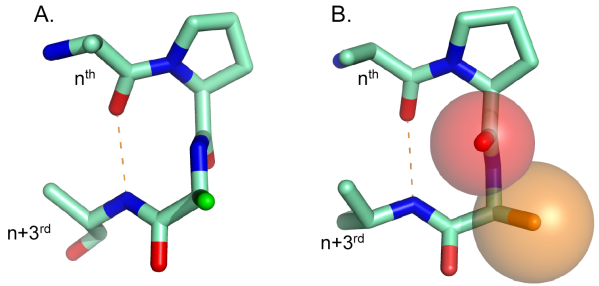
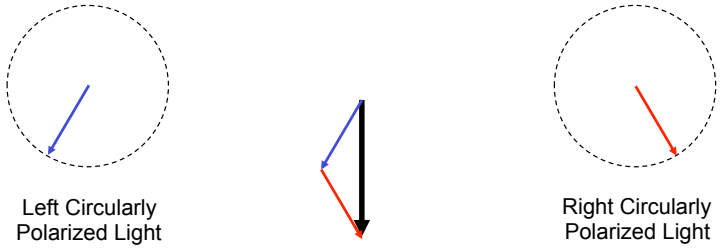


Figure 3.12. (A) Type I β turn and (B) Type II β turn. Note that the chief difference between them is the orientation of the peptide bond connecting residues n+1 to n+2. In the Type II turn, the side chain of the n+2nd residue is in steric conflict with the carbonyl oxygen of residue n+1. Thus, the n+2nd residue in Type II turns is often glycine.

Plane-Polarized Light



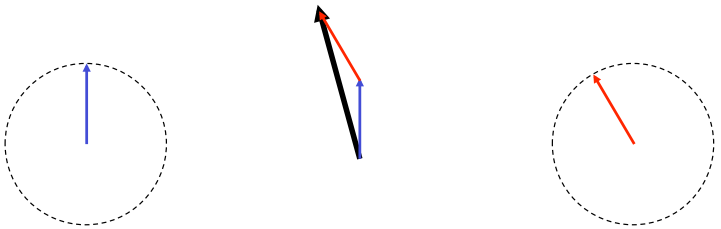
Left Circularly
Polarized Light

Right Circularly
Polarized Light

Equal populations of both
Forms of polarized light create
That oscillate in a plane

Good demo: http://www.enzim.hu/~szia/cddemo/edemo7.htm

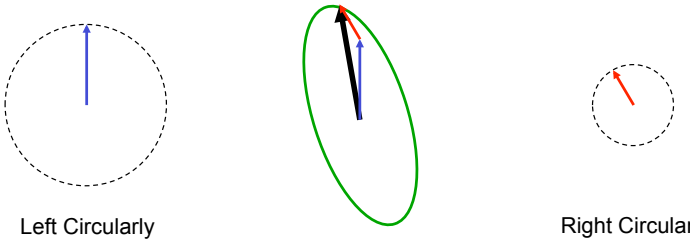
Optical Rotation



Left Circularly Polarized Light

Right Circularly Polarized Light – Retarded by Chiral compound, fields now sum to give rotated plane of polarization

Circular Dichroism

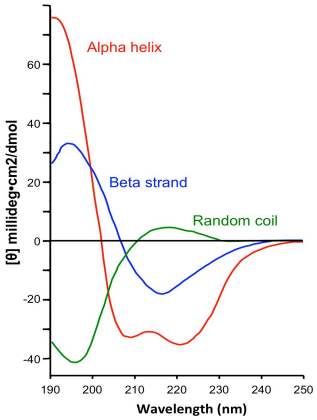


Left Circularly Polarized Light

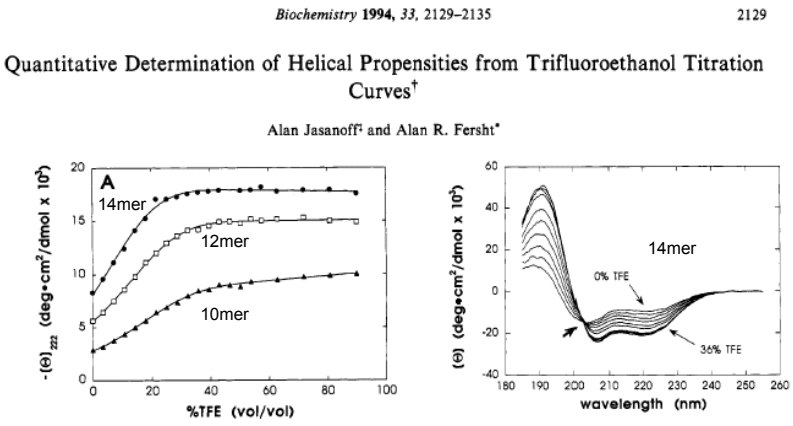
Right Circularly Polarized Light – Retarded and absorbed by Chiral Compound

CD Spectra of 2^{o} Structure

θ = ellipticity
[θ] = molar ellipticity
[θ] = 3298(ε_L-ε_R)



Helix stabilization by TFE



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Quantitative Determination of Helical Propensities from Trifluoroethanol Titration Curves†

Alan Jasanoff‡ and Alan R. Fersht*

Increased negative ellipticity [θ] at 222 nm indicates greater helix content in increasing concentrations of trifluoroethanol.