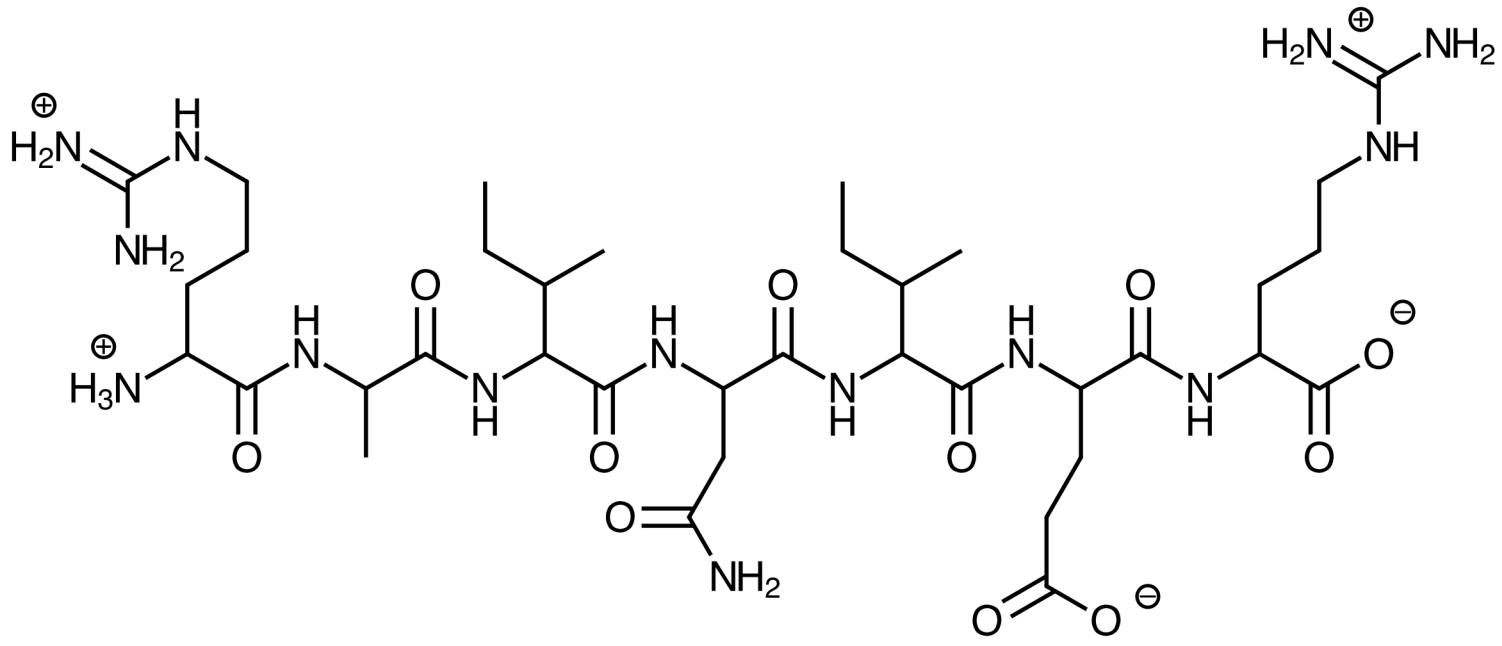
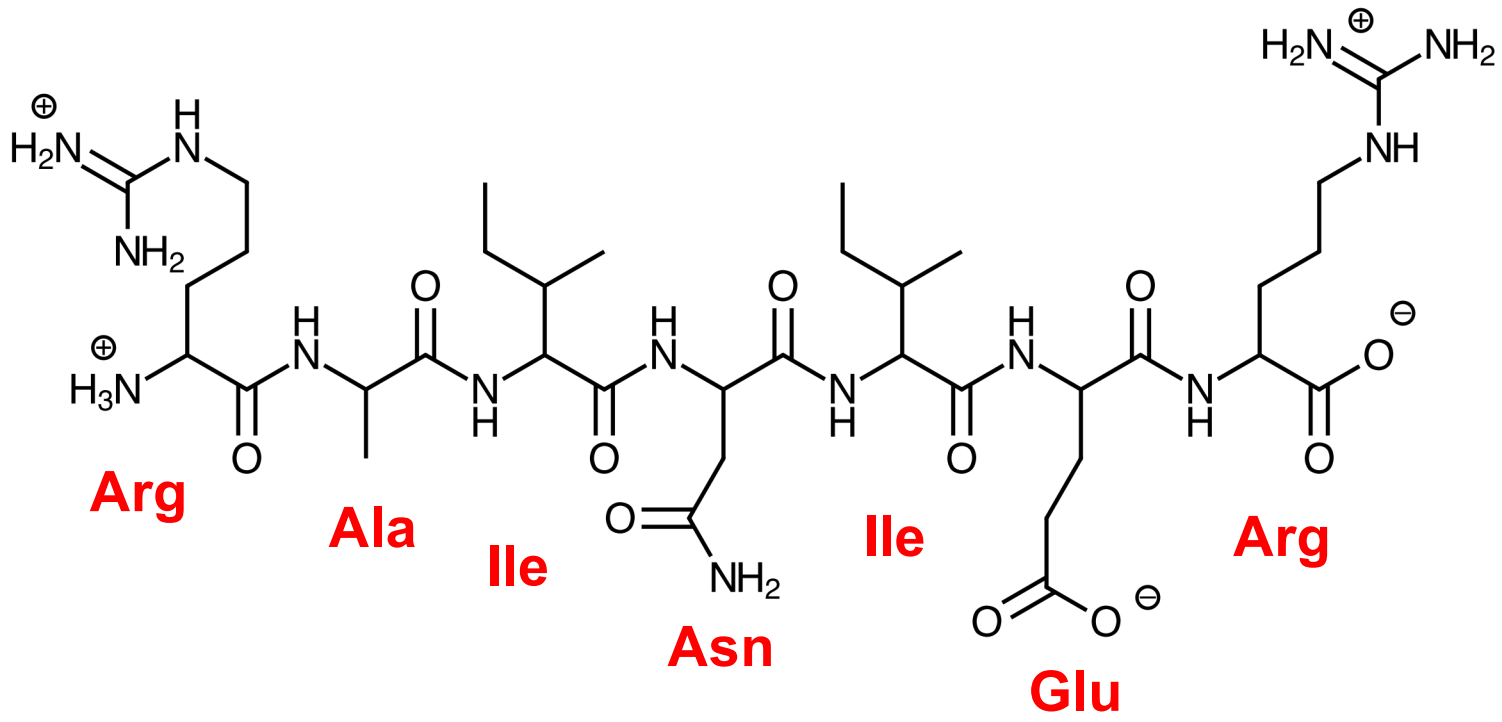
Who Am I?



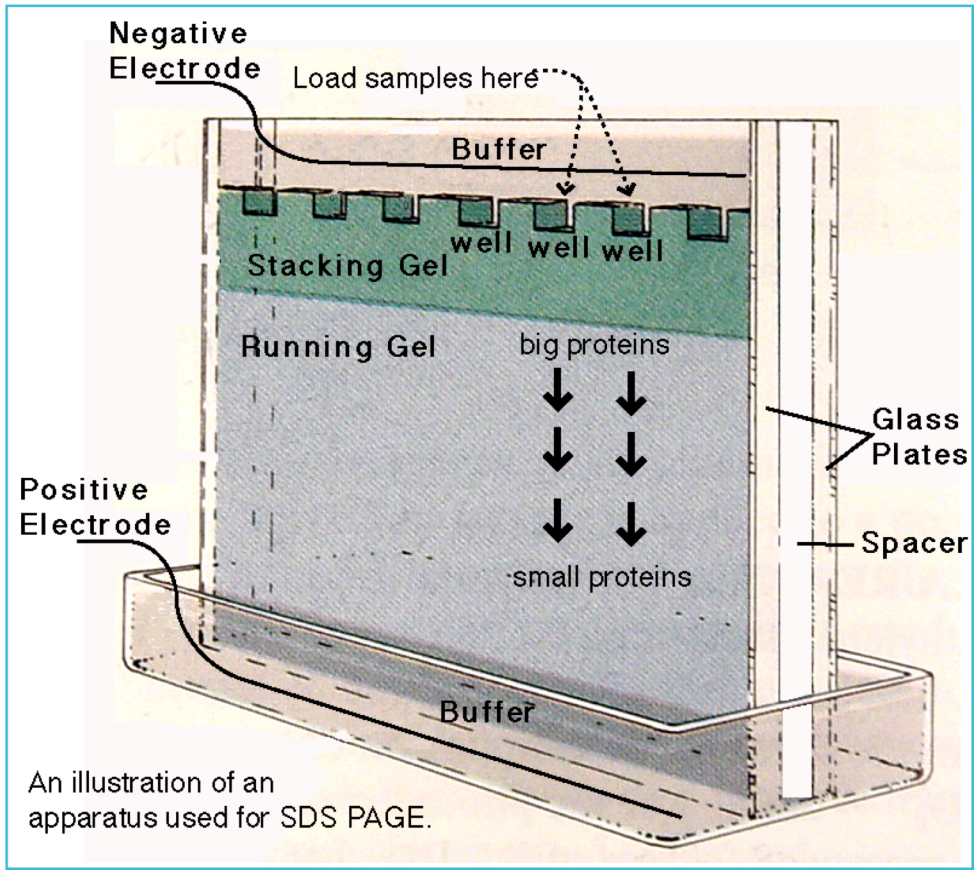
…and who geeked out this week?

Who Am I?

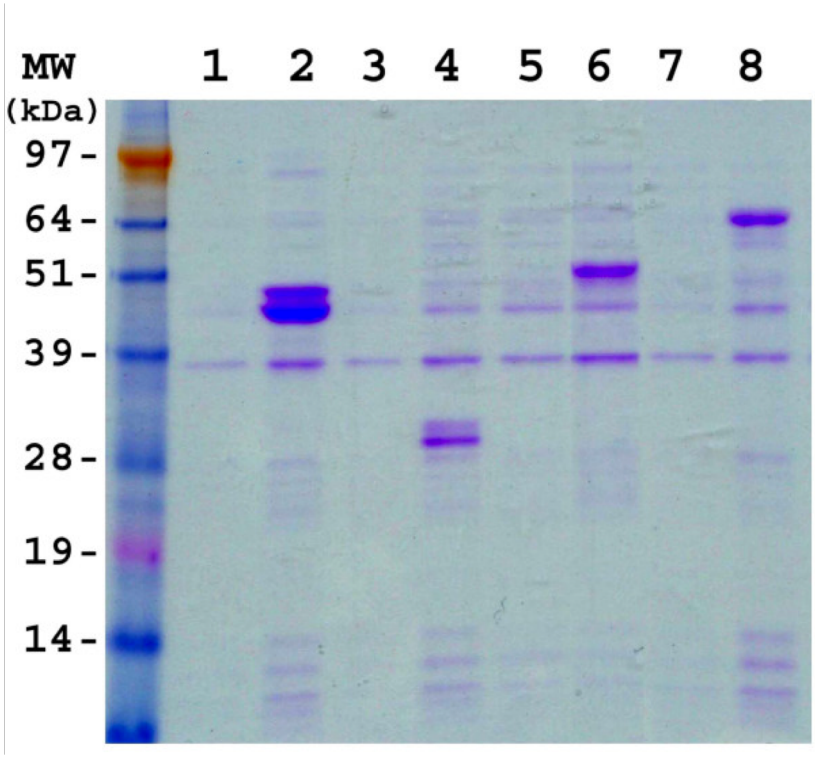


…and who geeked out this week?

Denaturing Polyacrylamide Gel Electrophoresis

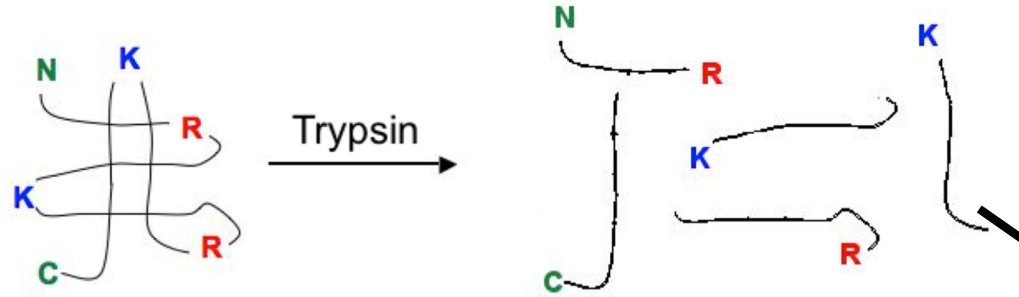


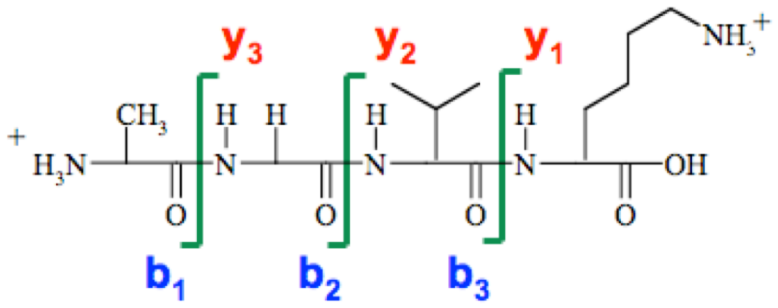
https://ww2.chemistry.gatech.edu/~lw26/bCourse_Information/4581/techniques/gel_elect/page_protein.html

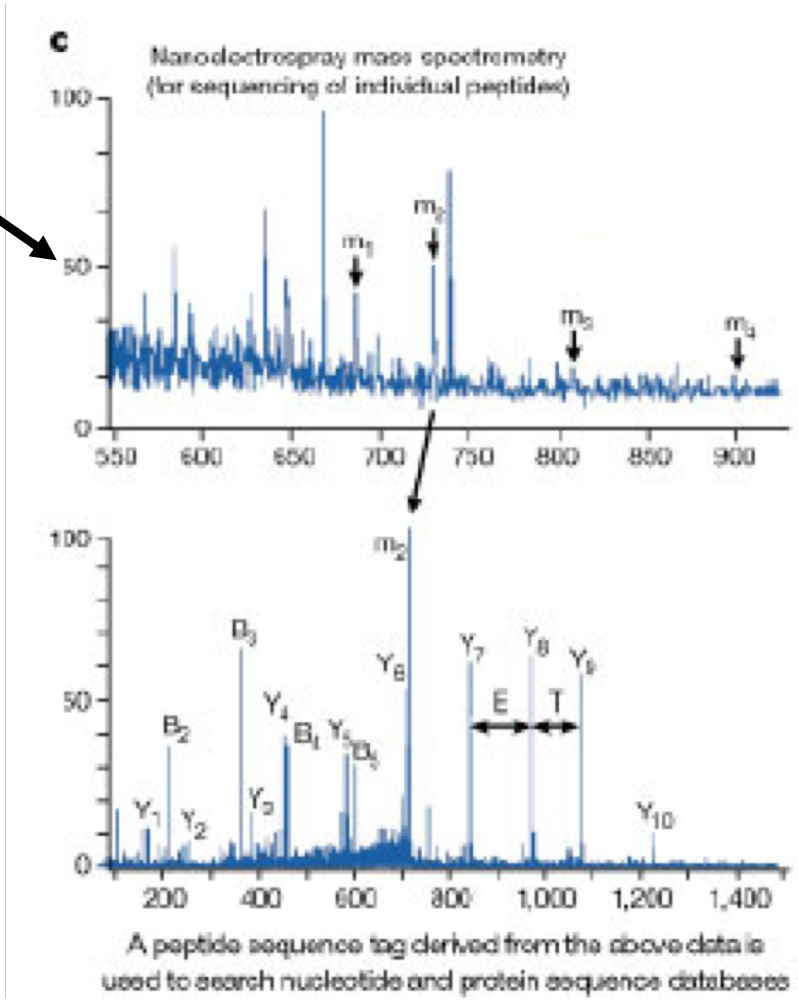


http://www.clinicalmolecularallergy.com/content/4/1/12/figure/F1

MS/MS Sequencing

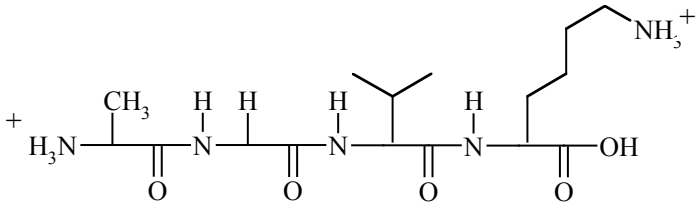




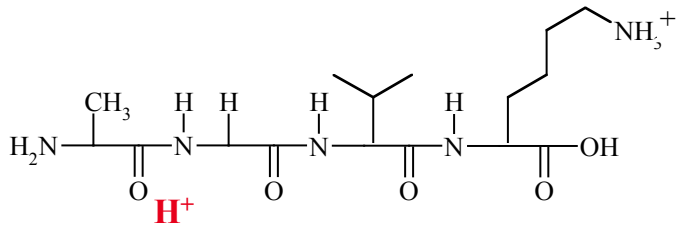


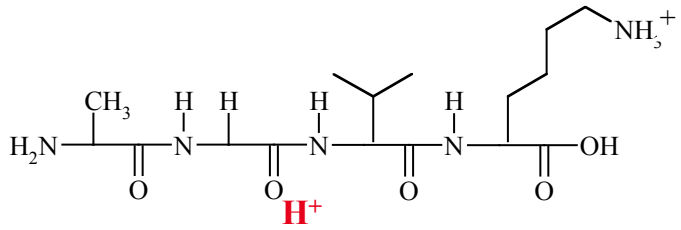
Migration of N-terminal Proton

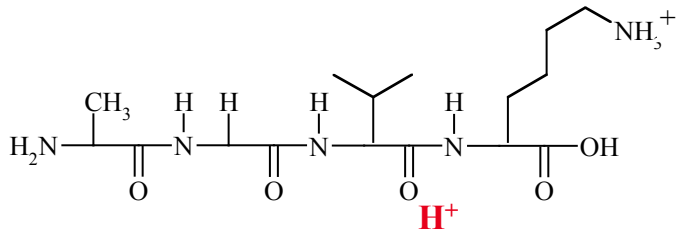
Mass =		
	Ala	71.0
	Gly	57.0
	Val	99.1
	Lys	128.1
	OH	17.0
	3 H^+	3.0
		375.2



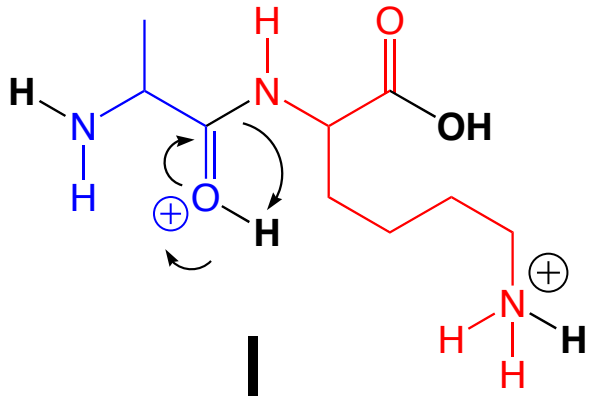
m/z = 375.2/2 = 187.6





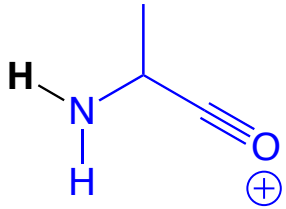


Collisionally Induced Dissociation



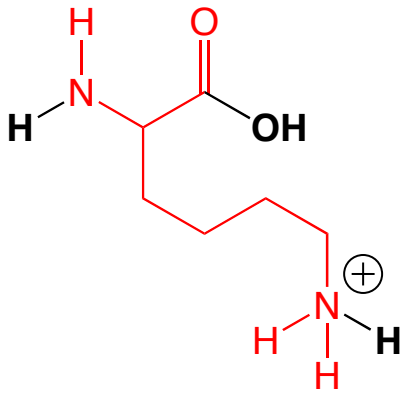
b_1: Ala 71.1
H^+ 1.0

72.1



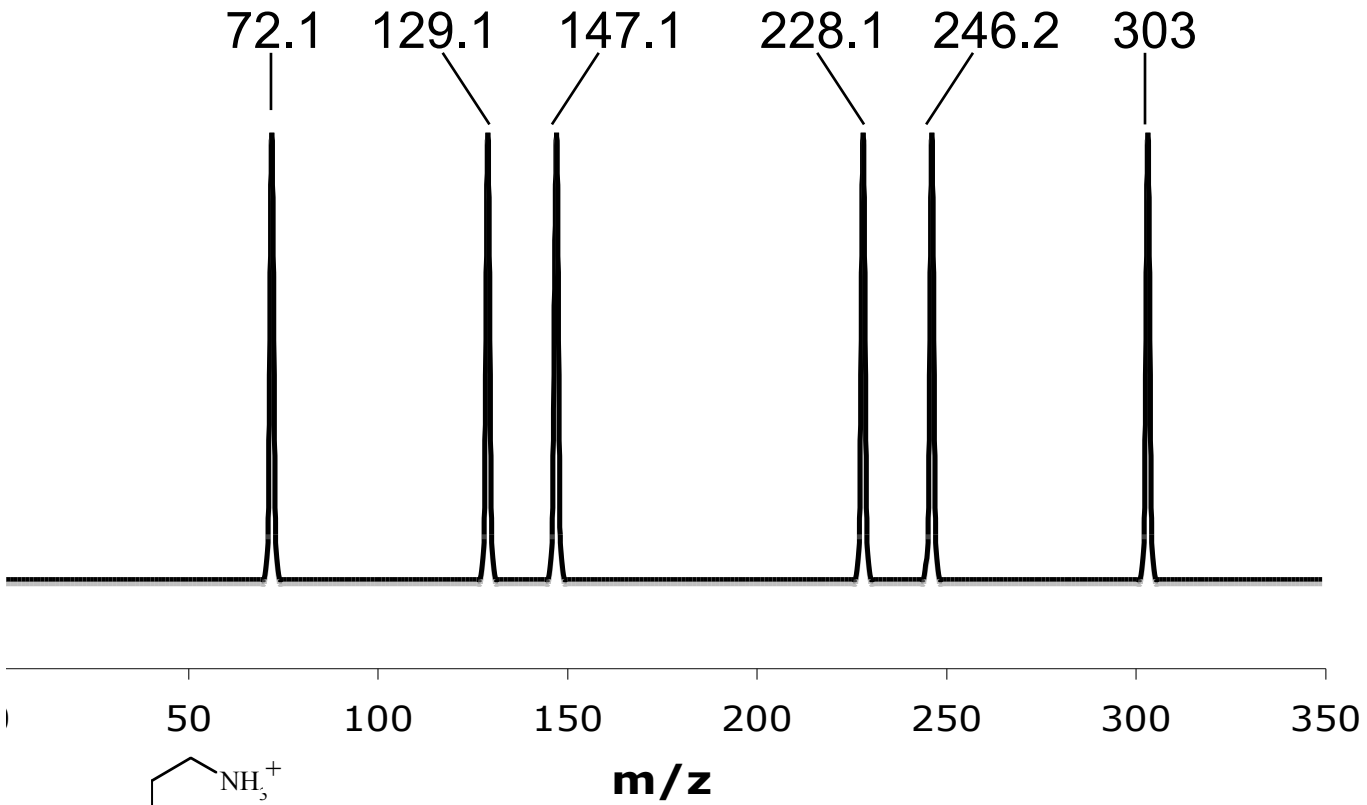
y_1: Lys 128.1
$2H^+$ 2.0
OH 17.0

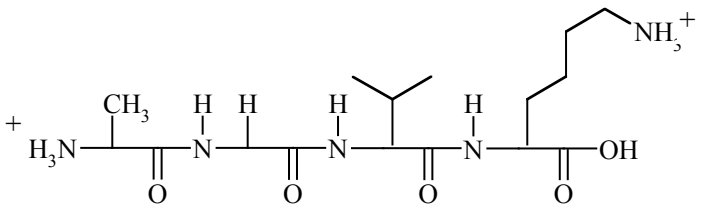
147.1



Fragment Spectrum of AGVK

m/z = 375.2/2 = 187.6

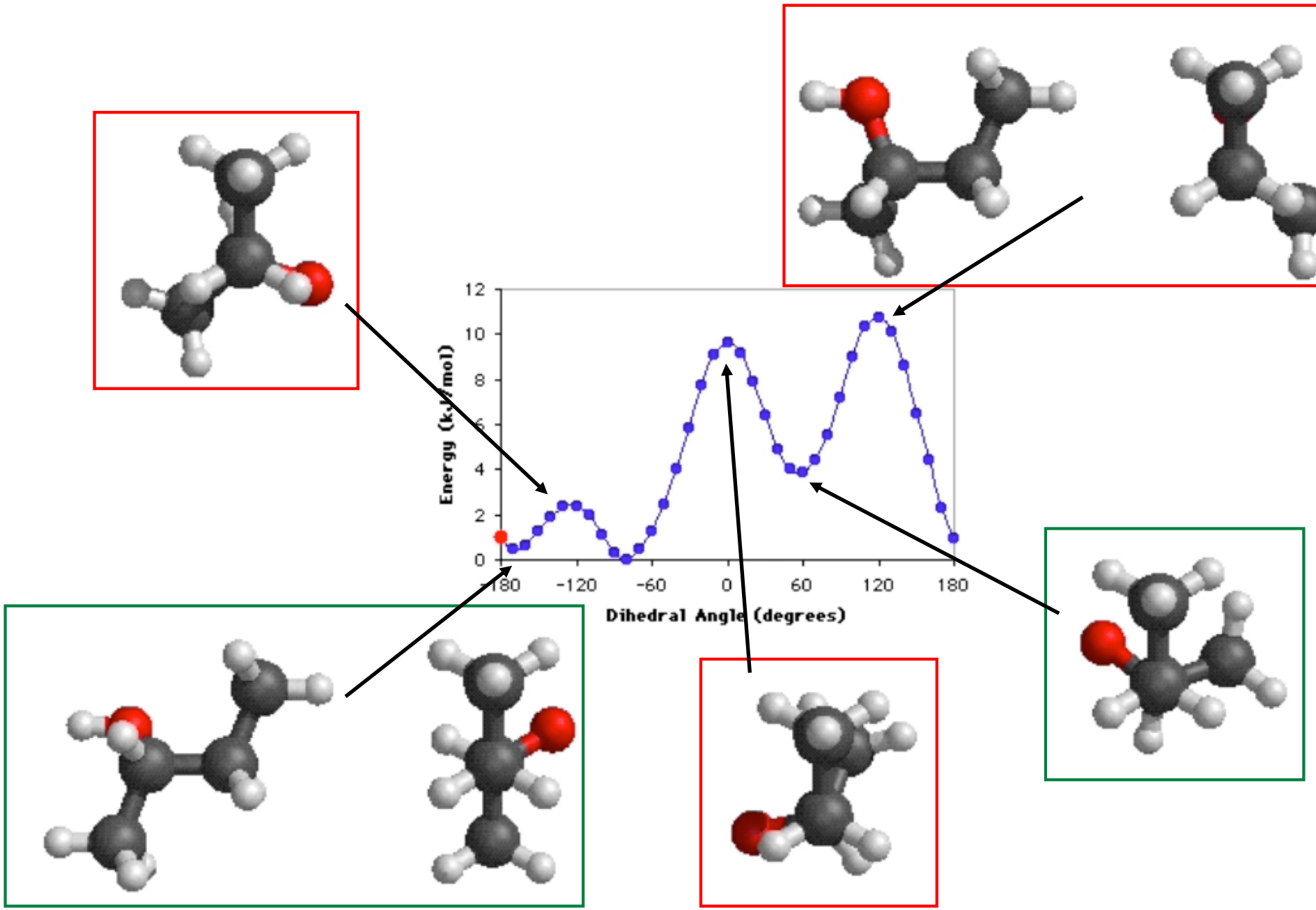




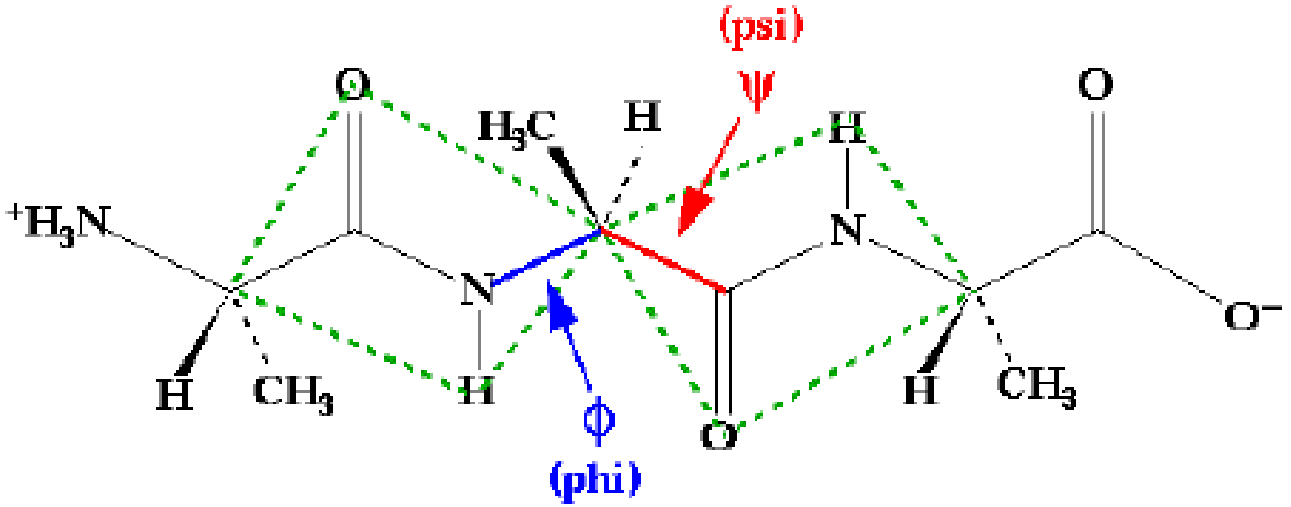
Properties of the Twenty

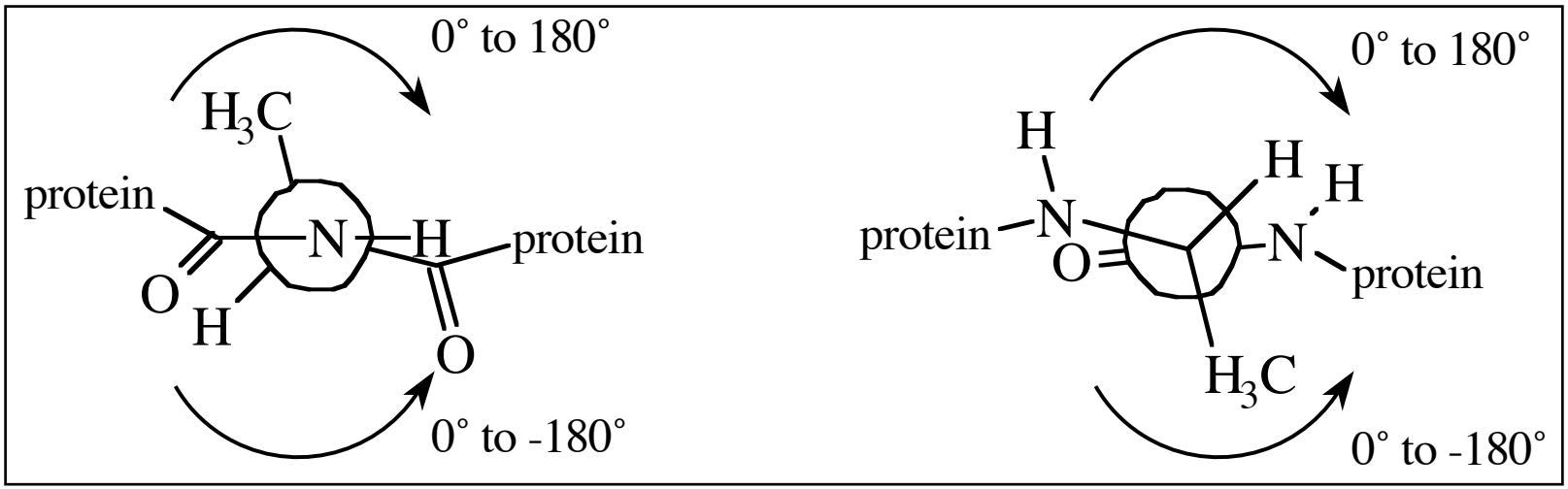
Amino Acid	Abbreviations	Residue Mass (Da)	Side Chain pK_a	$\Delta\Delta G^{\circ}$ transfer (kcal/mol)
Alanine	Ala, A	71.09	-	-0.87
Arginine	Arg, R	156.19	**12**	15.93
Asparagine	Asn, N	114.11	-	5.22
Aspartic Acid	Asp, D	115.09	**4**	9.71
Cysteine	Cys, C	103.15	**8**	-0.34
Glutamine	Gln, Q	128.14	-	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

S-2-Butanol Conformers

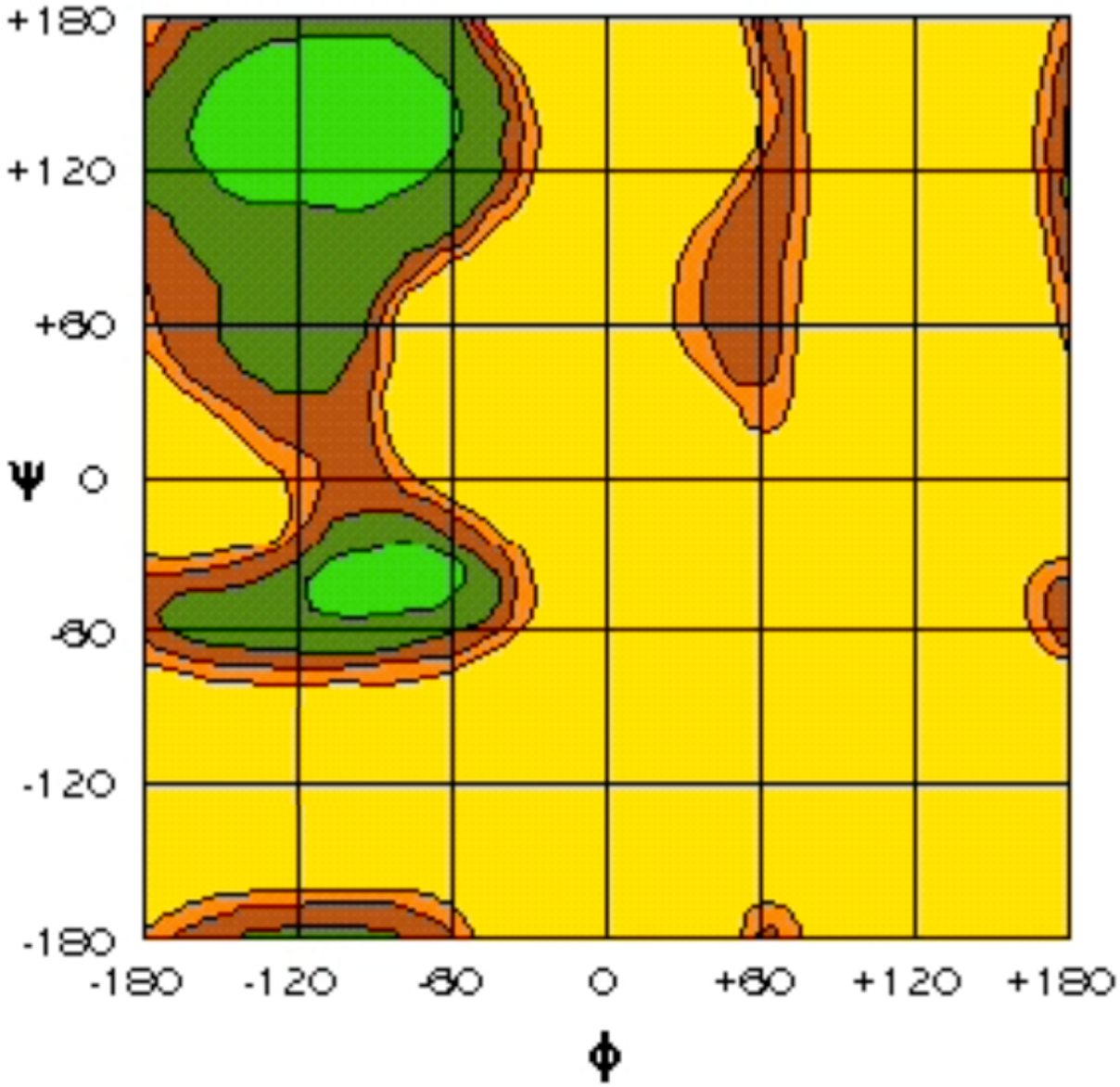


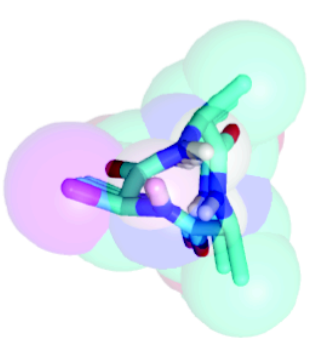
Phi (ϕ) and Psi (ψ) Dihedrals



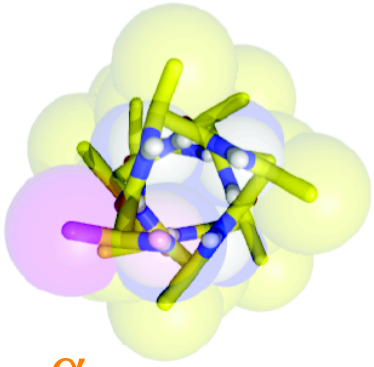


Ramachandran plot

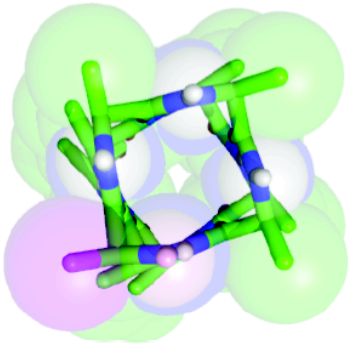




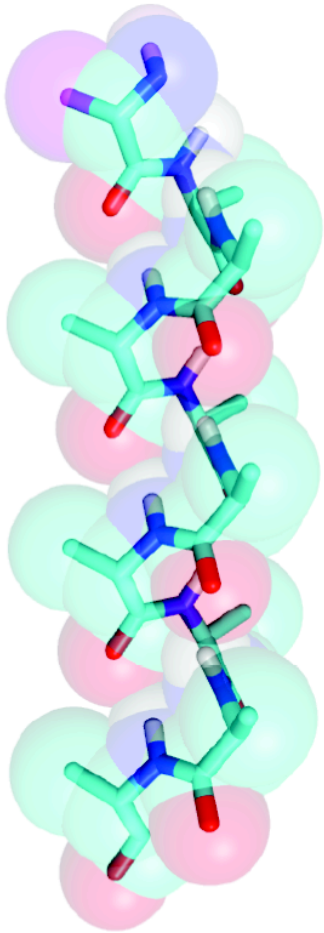
3_{10}



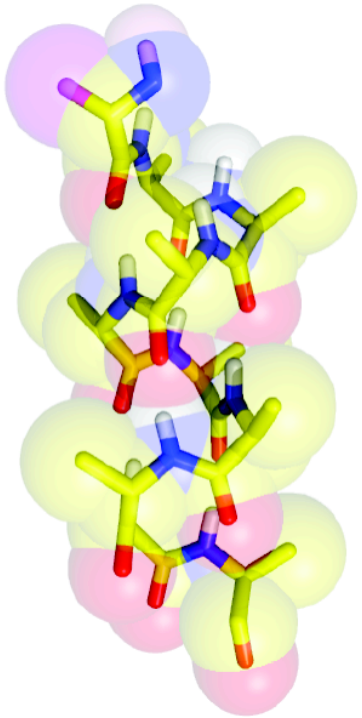
α



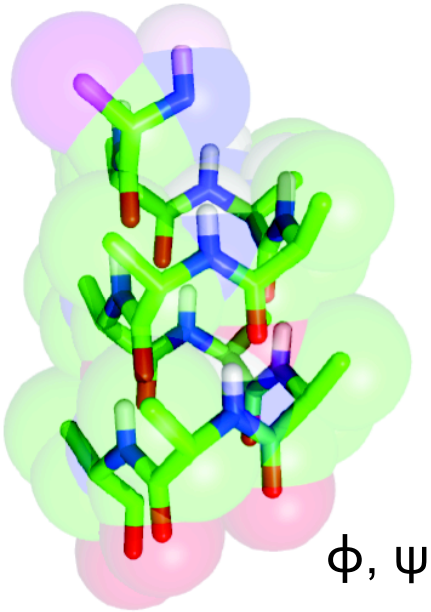
π



ϕ, ψ = -74º, -4º

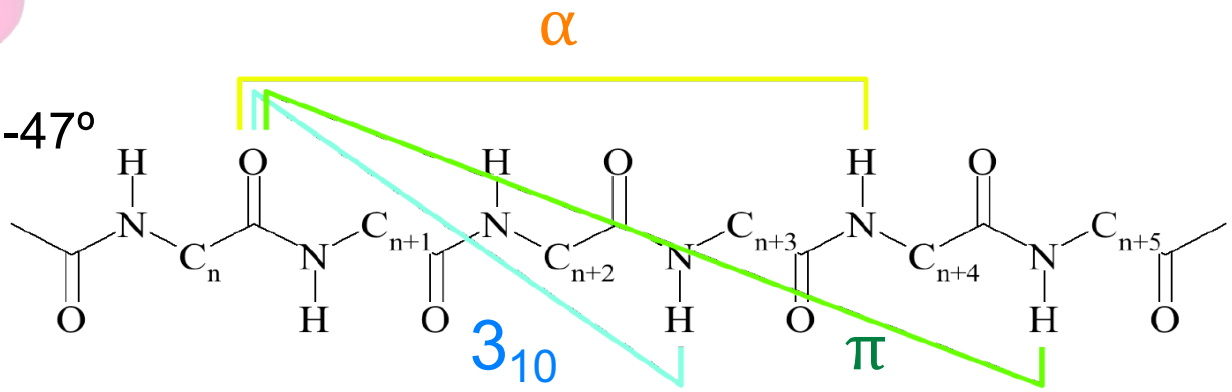


ϕ, ψ = -56º, -47º

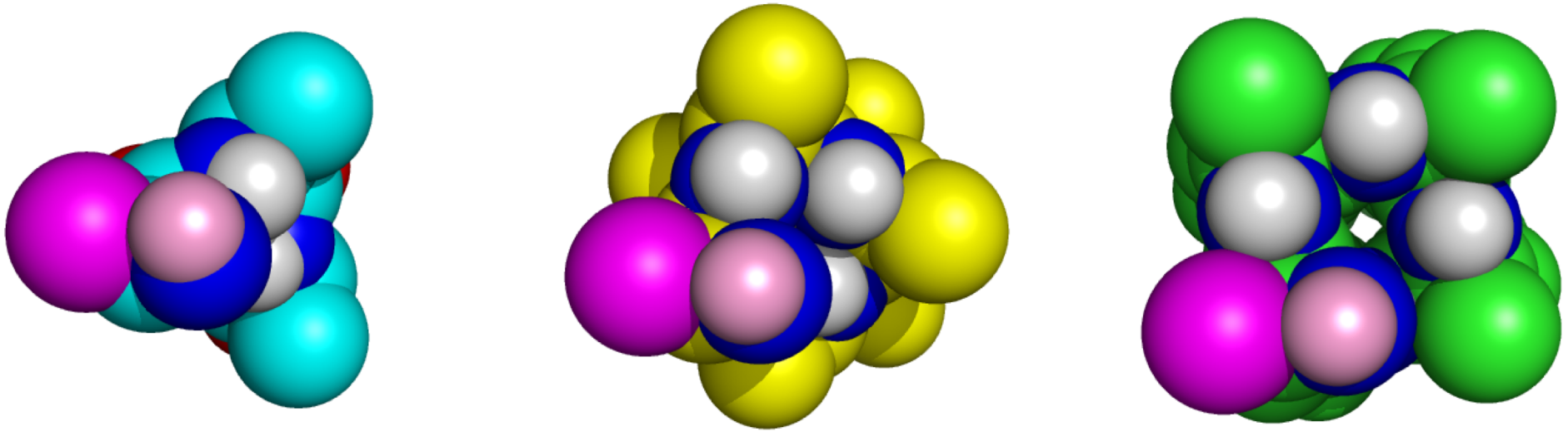


ϕ, ψ = -59º, -70º

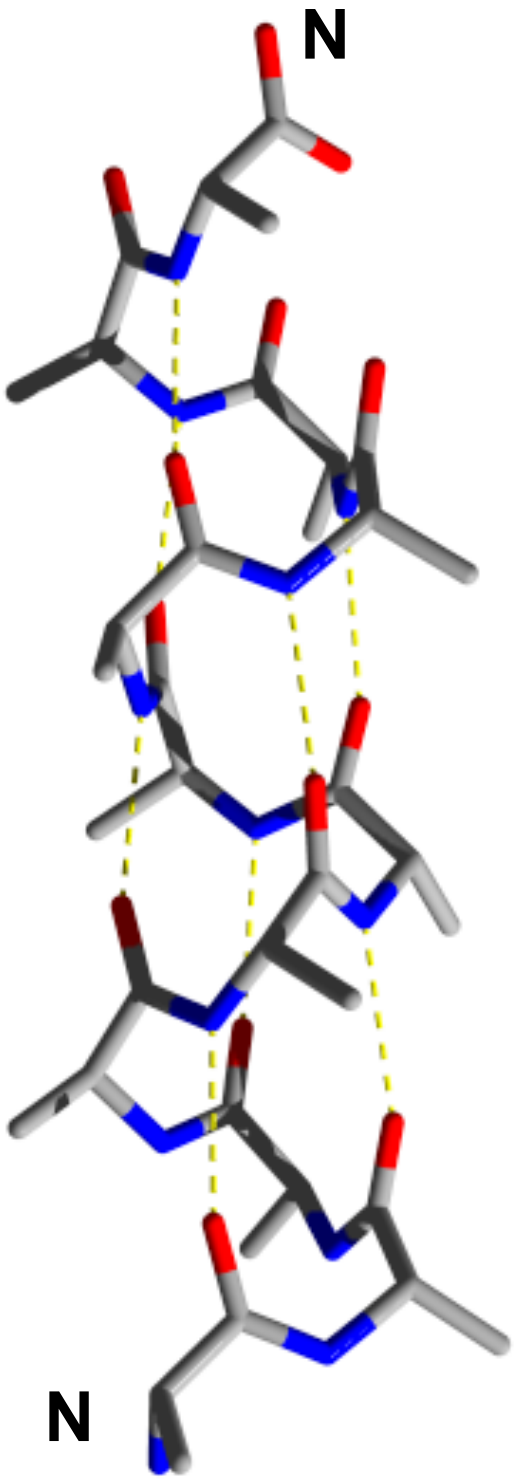
Three Possible Right-handed Helices



Three Helices



3_{10} α π



α-Helix Statistics

Right-handed twist

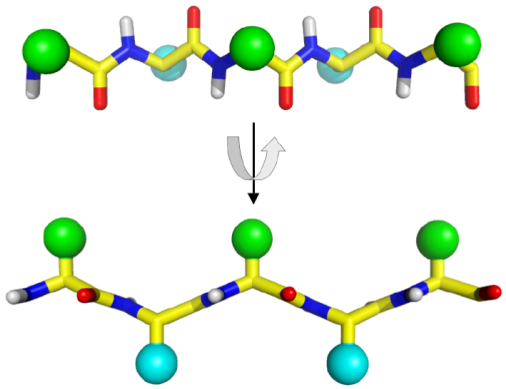
ϕ, ψ = -47˚, -57˚
3.6 residues/turn

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

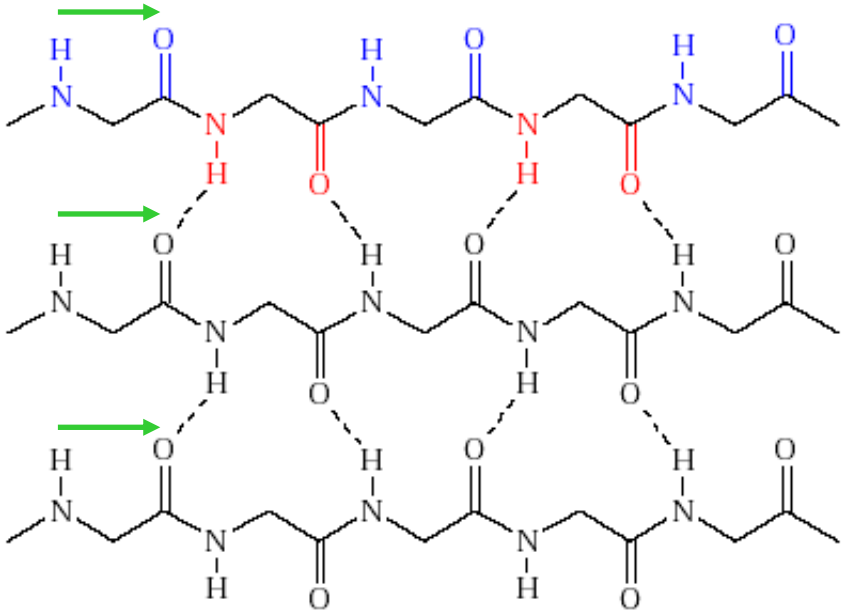
Helix diameter = 4.6 Å

Beta Strands

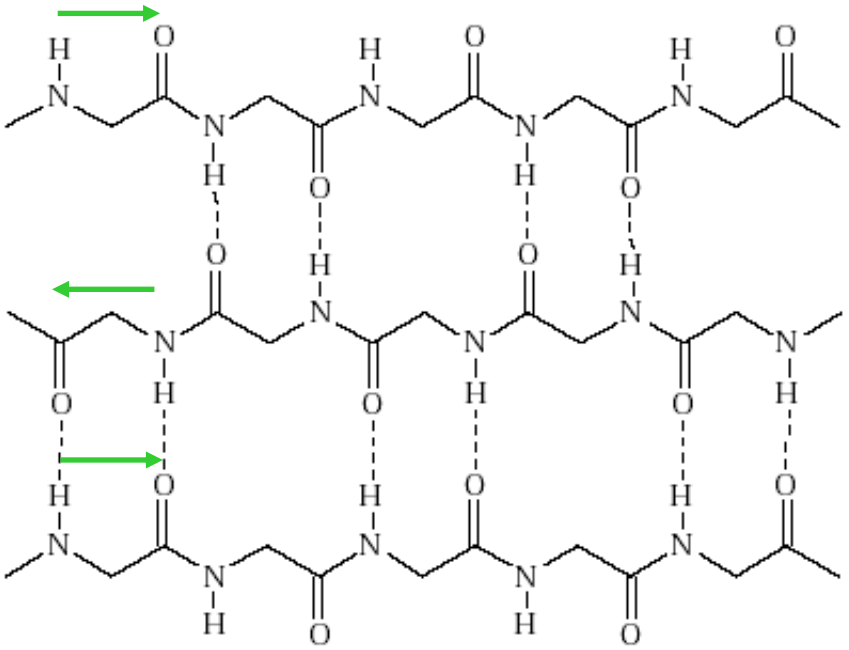
$\phi \approx -120^\circ$ to -140°, $\psi = 110^\circ$ to 130°



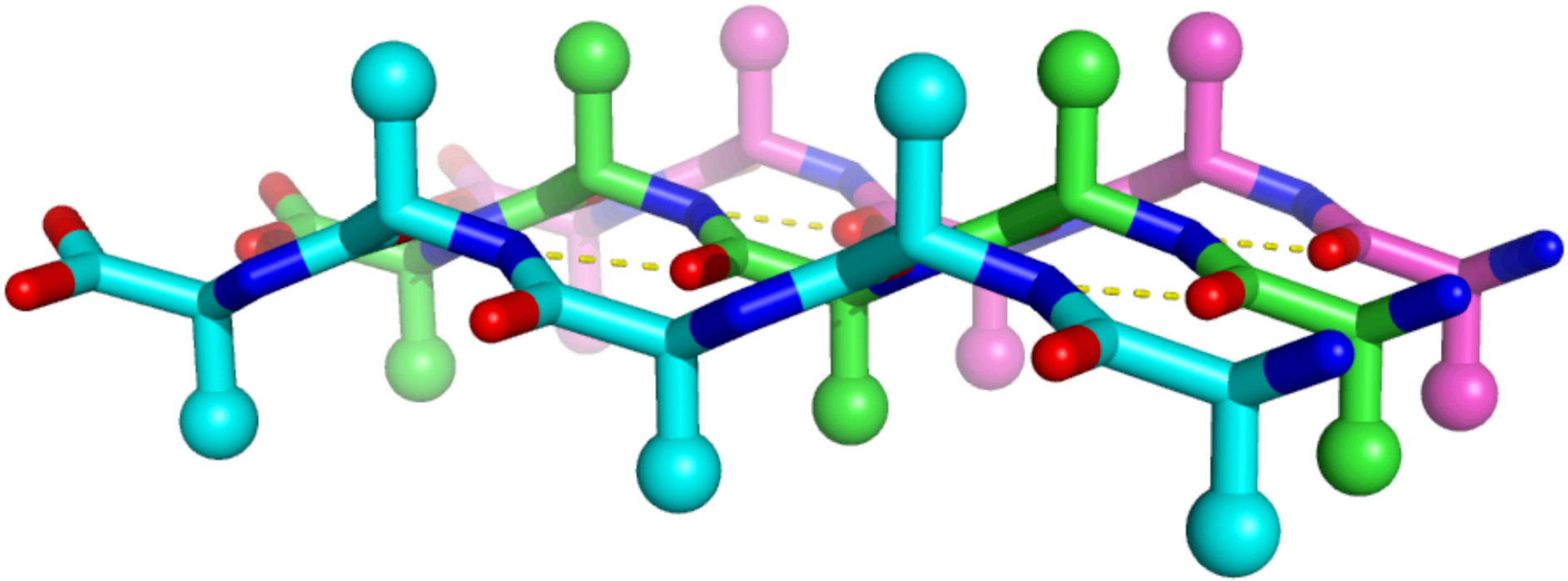
Parallel β–Sheet



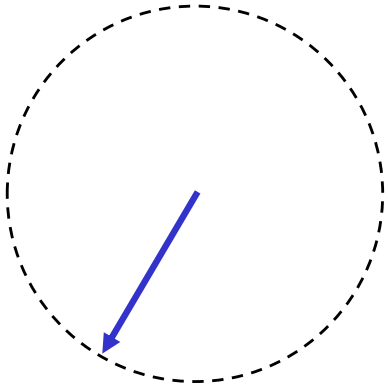
Antiparallel β-Sheet



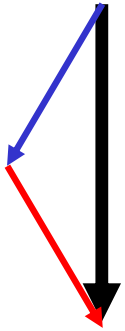
Beta Pleated Sheet

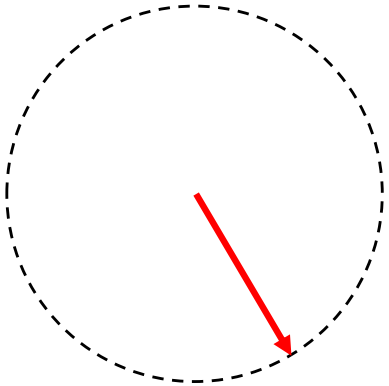


Plane-Polarized Light



Left Circularly
Polarized Light



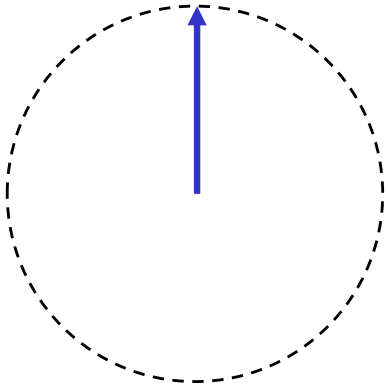


Right Circularly
Polarized Light

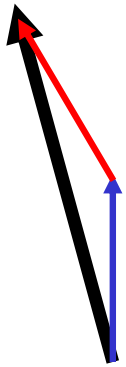
Equal populations of both
Forms of polarized light create
That oscillate in a plane

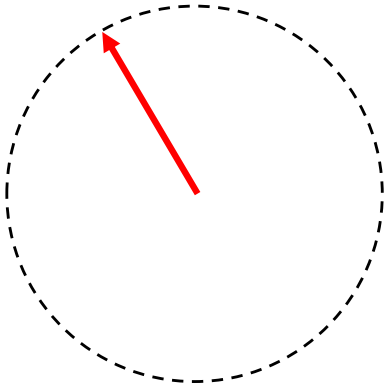
Good demo: http://www.enzim.hu/~szia/cddemo/edemo7.htm

Optical Rotation



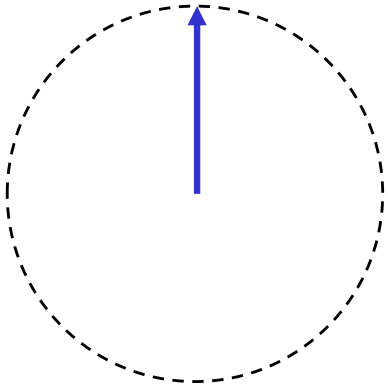
Left Circularly Polarized Light



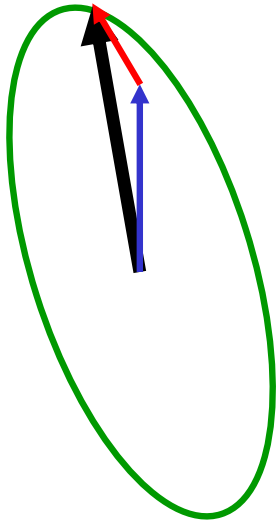


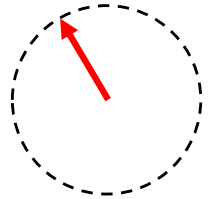
Right Circularly Polarized Light – Retarded by Chiral compound, fields now sum to give rotated plane of polarization

Circular Dichroism



Left Circularly
Polarized Light





Right Circularly
Polarized Light –
Retarded and absorbed
by Chiral
Compound

CD Spectra of 2^{o} Structure

θ = ellipticity
$[\theta]$ = molar ellipticity
$[\theta] = 3298(\varepsilon_L - \varepsilon_R)$