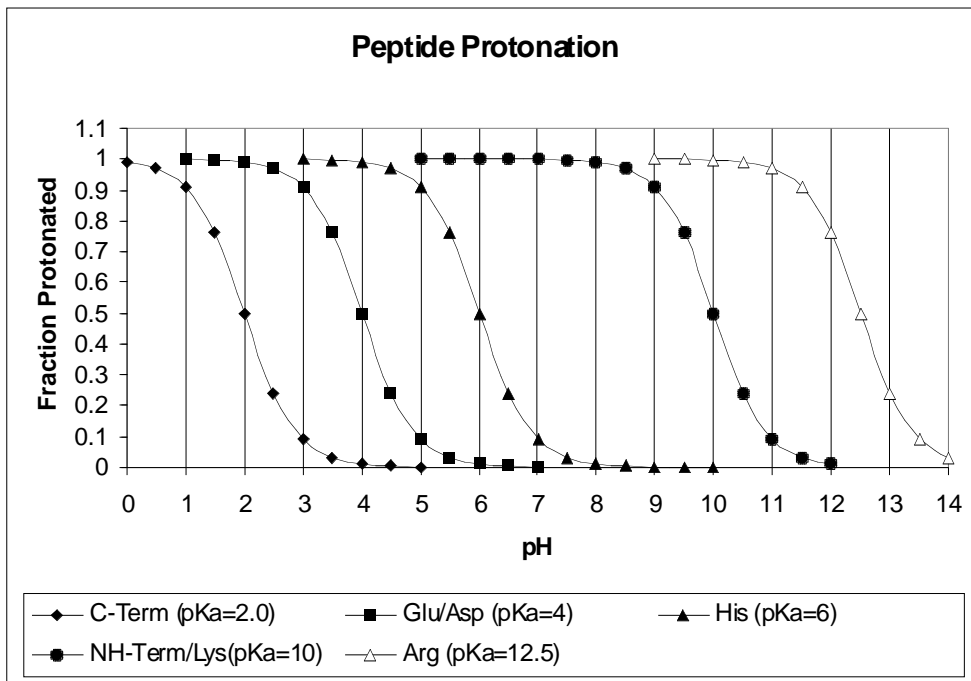


Ionizable Amino Acids/Protonated - deprotonated forms

	Protonated (pH << pKa)	Deprotonated (pH >> pKa)
Carboxy-Terminus pKa=2		
Amino-Terminus pKa=10		
Aspartic Acid (Asp) pKa=4		
Glutamic Acid (Glu) pKa=4		
Histidine (His) pKa=6		
Lysine (Lys) pKa=10		
Arginine (Arg) pKa=12.5		
Cysteine (Cys) pKa=8		
Tyrosine (Tyr) pKa=10		



Some useful Formula:

$$pH = pK_A + \log([A^-]/[HA])$$

$$pH = pK_A + \log(R)$$

$$pH - pK_A = \log(R)$$

$$10^{pH - pK_A} = R$$

$$[A^-]/[HA] = R$$

$$[A^-] = [HA]R$$

$$[A_T] = [A^-] + [HA]$$

$$[A_T] = [HA](1 + R)$$

$$[HA] = [A_T] \frac{1}{(1 + R)}$$

$$[A^-] = [A_T] \frac{R}{(1 + R)}$$

Key Landmarks:

- pH is 2 units lower than pKa: $F_{HA} \approx 0.99$
- pH is 1 unit lower than pKa: $F_{HA} \approx 0.90$
- pH is equal to the pKa: $F_{HA} \approx 0.50$
- pH is 1 unit higher than pKa: $F_{HA} \approx 0.10$
- pH is 2 units higher than pKa: $F_{HA} \approx 0.01$

Using the ionization of the side chain of Histidine as an example (pKa=6.0)

pH	R	F _{HA}
4	$R = 10^{(4-6)} = 10^{-2}$	$F_{HA} = 1/(1 + 0.01) = 0.99$
5	$R = 10^{(5-6)} = 10^{-1}$	$F_{HA} = 1/(1 + 0.10) = 0.91$
6	$R = 10^{(6-6)} = 10^0$	$F_{HA} = 1/(1 + 1) = 0.50$
7	$R = 10^{(7-6)} = 10^{+1}$	$F_{HA} = 1/(1 + 10) = 0.091$
8	$R = 10^{(8-6)} = 10^{+2}$	$F_{HA} = 1/(1 + 100) = 0.01$