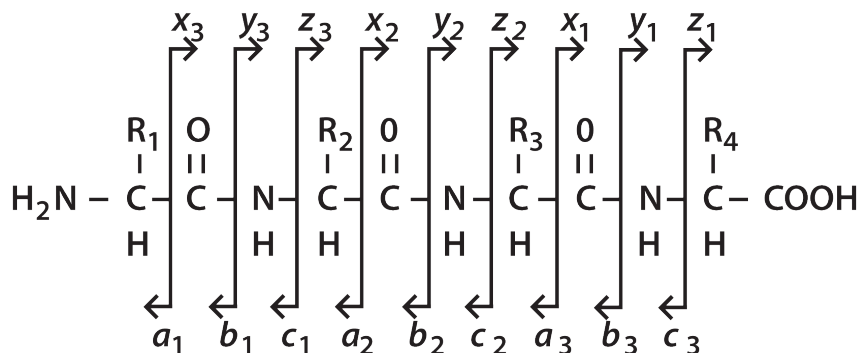


Structural analysis (CH-314)

Week 4

Definitions & Formulas

1. Peptide fragmentation nomenclature:



2. Mass of a peptide (in its neutral form):

$$M = m(H_2O) + \sum_{i=1}^N m(R_i + C_2H_2NO)$$

3. Mass-to-charge ratio of b/y fragments:

$$m/z(b_k^{q+}) = \frac{\sum_{i=1}^{k-1} m(R_i + C_2H_2NO) + m(R_k) + m(C_2H_2NO) + q \cdot m(H^+)}{q}$$

$$m/z(y_k^{q+}) = \frac{\sum_{i=1}^{k-1} m(R_i + C_2H_2NO) + m(R_k) + m(C_2H_4NO_2) + q \cdot m(H^+)}{q}$$

4. Masses of an electron and of a proton:

$$m_e = 0.000549 \text{ Da}$$

$$m(H^+) = 1.007276 \text{ Da}$$

Standard Amino Acids

Amino acid		Side chain (R)	Monoisotopic mass (Da)		pK _a		
			R	R + C ₂ H ₂ NO	N-term	C-term	R
Glycine	Gly (G)	H	1.007825	57.021464	9.60	2.34	-
Alanine	Ala (A)	CH ₃	15.023475	71.037114	9.69	2.34	-
Serine	Ser (S)	CH ₃ O	31.018390	87.032028	9.15	2.21	-
Proline	Pro (P)	C ₃ H ₅	41.039125	97.052764	10.60	1.99	-
Valine	Val (V)	C ₃ H ₇	43.054775	99.068414	9.62	2.32	-
Threonine	Thr (T)	C ₂ H ₅ O	45.034040	101.048678	9.10	2.09	-
Cysteine	Cys (C)	CH ₃ S	46.995546	103.009185	10.28	1.96	8.18
Leucine	Leu (L)	C ₄ H ₉	57.070425	113.084064	9.60	2.36	-
Isoleucine	Ile (I)	C ₄ H ₉	57.070425	113.084064	9.60	2.36	-
Asparagine	Asn (N)	C ₂ H ₄ NO	58.029289	114.042927	8.80	2.02	-
Aspartic acid	Asp (D)	C ₂ H ₃ O ₂	59.013304	115.026943	9.60	1.88	3.65
Glutamine	Gln (Q)	C ₃ H ₆ NO	72.044939	128.058578	9.13	2.17	-
Lysine	Lys (K)	C ₄ H ₁₀ N	72.081324	128.094963	8.95	2.18	10.53
Glutamic acid	Glu (E)	C ₃ H ₅ O ₂	73.028954	129.042593	9.67	2.19	4.25
Methionine	Met (M)	C ₃ H ₇ S	75.026846	131.040485	9.21	2.28	-
Histidine	His (H)	C ₄ H ₅ N ₂	81.045273	137.058912	9.17	1.82	6.00
Phenylalanine	Phe (F)	C ₇ H ₇	91.054775	147.068414	9.13	1.83	-
Arginine	Arg (R)	C ₄ H ₁₀ N ₃	100.087472	156.101111	9.04	2.17	12.48
Tyrosine	Tyr (Y)	C ₇ H ₇ O	107.049690	163.063329	9.11	2.20	10.07
Tryptophan	Trp (W)	C ₉ H ₈ N	130.065674	186.079313	9.39	2.83	-