

This script calculates molar absorptivities (extinction coefficients) at 205 nm and 280 nm from an amino acid sequence. It also calculates the molecular weight for various universal isotopic labeling schemes.

Reference:

Anthis N.J., Clore G.M. (2013) Sequence-specific determination of protein and peptide concentrations by absorbance at 205 nm, Protein Science in press, epub ahead of publication doi:10.1002/pro.2253

Amino acid sequence:

GASSDIQVKELEKRASGQAFELILSPRSKESVPEFPLSPPKKDLSELEIQKKLEAABERRKSHAEVLKQLAEKREHEKEVLQKAIENNPFKMAEKLTHKMEANKENREAQMAAKLERLREKDKHIEEVRKNKESKDPADETED

Number of residues:

149

Molecular weight (in H2O):

natural abundance	17228.02
2H	18143.80
13C	17959.12
15N	17445.56
2H,13C	18874.89
2H,15N	18361.33
13C,15N	18176.65
2H,13C,15N	19092.43

Amino acid composition:

A = 15
C = 0
D = 6
E = 30
F = 3
G = 2
H = 4
I = 5
K = 23
L = 13
M = 3
N = 6
P = 6
Q = 6
R = 9
S = 11
T = 2
V = 5
W = 0
Y = 0

Atomic composition:

Carbon (C)	739
Hydrogen (H)	1227
non-exchangeable	923
exchangeable	304
Nitrogen (N)	219
Oxygen (O)	247
Sulfur (S)	3

Molar absorptivity (extinction coefficient) at 280 nm = 0 M-1 cm-1

Molar absorptivity (extinction coefficient) at 205 nm = 480480 M-1 cm-1