

# The isoelectric point of a protein

an excel (3.0a) worksheet by L.H. Oestergaard © 1994.

Instruction: Worksheet for calculation of the theoretical pI value for a protein.  
Simple fill in the boxed cells with your data and watch the magic!!!

Protein:

Amino acid	pK (carboxyl grp.)	pK (amino grp.)	pK (side chain)	No. of residues
<b>Ala</b>	2.3	9.7		
<b>Arg</b>	2.2	9	12.5	<input type="text" value="10"/>
<b>Asn</b>	2	8.8		
<b>Asp</b>	2.1	9.8	3.9	<input type="text" value="18"/>
<b>Cys</b>	1.7	10.8	8.3	<input type="text" value="5"/>
<b>Gln</b>	2.2	9.1		
<b>Glu</b>	2.2	9.7	4.3	<input type="text" value="15"/>
<b>Gly</b>	2.3	9.6		
<b>His</b>	1.8	9.2	6	<input type="text" value="6"/>
<b>Ile</b>	2.4	9.7		
<b>Leu</b>	2.4	9.6		
<b>Lys</b>	2.2	9	10.5	<input type="text" value="26"/>
<b>Met</b>	2.3	9.2		
<b>Phe</b>	1.8	9.1		
<b>Pro</b>	2	10.6		
<b>Ser</b>	2.2	9.2		
<b>Thr</b>	2.6	10.4		
<b>Trp</b>	2.4	9.4		
<b>Tyr</b>	2.2	9.1	10.1	<input type="text" value="11"/>
<b>Val</b>	2.3	9.6		

pK value of the N-terminal amino acid (see table above):   
pK value of the C-terminal amino acid (see table above):

The number of protonated residues of a specific amino acid is determined by the equation

$$N_p = N_t \cdot [H^+] / ([H^+] + K_N)$$

where  $N_p$ =no. of protonated residues,  $N_t$ =total no. of residues of the specific amino acid,  
 $[H^+] = 10^{-(pH)}$ ,  $K$ =dissociation const. for the specific amino acid ( $=10^{-(pK)}$ ).

\*\*\* Please note that a protonated basic amino acid actually is not charged. \*\*\*

Protein: Glyceraldehyde-3-phosphate dehydrogenase from mouse

<b>pH</b>	<b>No. of neg. charges</b>	<b>No. of pos. charges</b>	<b>Net. charge</b>
1.00	0	43	43
1.50	0	43	43
2.00	-1	43	42
2.50	-2	43	41
3.00	-4	43	39
3.50	-8	43	35
4.00	-16	43	27
4.50	-25	43	18
5.00	-30	42	12
5.50	-33	42	9
6.00	-34	40	6
6.50	-34	38	4
7.00	-34	38	3
7.50	-35	37	2
8.00	-36	37	1
8.50	-37	37	-1
9.00	-39	36	-3
9.50	-41	34	-7
10.00	-44	30	-14
10.50	-47	23	-24
11.00	-49	16	-33
11.50	-50	11	-38
12.00	-50	8	-41
12.50	-50	5	-45
13.00	-50	2	-48



Np (Lys)	Np (Arg)	Np (His)	Np (Tyr)	Np (Cys)	Np (Glu)	Np (Asp)
26	10	6	0	0	0	0
26	10	6	0	0	0	0
26	10	6	0	0	0	0
26	10	6	0	0	0	1
26	10	6	0	0	1	2
26	10	6	0	0	2	5
26	10	6	0	0	5	10
26	10	6	0	0	9	14
26	10	5	0	0	13	17
26	10	5	0	0	14	18
26	10	3	0	0	15	18
26	10	1	0	0	15	18
26	10	1	0	0	15	18
26	10	0	0	1	15	18
26	10	0	0	2	15	18
26	10	0	0	3	15	18
25	10	0	1	4	15	18
24	10	0	2	5	15	18
20	10	0	5	5	15	18
13	10	0	8	5	15	18
6	10	0	10	5	15	18
2	9	0	11	5	15	18
1	8	0	11	5	15	18
0	5	0	11	5	15	18
0	2	0	11	5	15	18

Np (N-term.) Np (C-term.)

1	0
1	0
1	0
1	1
1	1
1	1
1	1
1	1
1	1
1	1
1	1
1	1
1	1
1	1
1	1
1	1
1	1
1	1
1	1
1	1
0	1
0	1
0	1
0	1
0	1
0	1
0	1
0	1
0	1
0	1