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Mass Table *

Seq.	Mass	Seq.	Mass	Seq.	Mass	Seq.	Mass
A	71.0371	DT	216.0746	HH	274.1178	NR	270.1440
AA	142.0742	DV	214.0954	HK	265.1539	NS	201.0750
AC	174.0463	DW	301.1063	HL	250.1430	NT	215.0906
AD	186.0641	DY	278.0903	HM	268.0994	NV	213.1113
AE	200.0797	E	129.0426	HN	251.1018	NW	300.1223
AF	218.1055	EE	258.0852	HP	234.1117	NY	277.1063
AG	128.0586	EF	276.1110	HQ	265.1175	P	97.0528
AH	208.0960	EG	186.0641	HR	293.1600	PP	194.1055
AK	199.1321	EH	266.1015	HS	224.0909	PQ	225.1113
AL	184.1212	EK	257.1375	HT	238.1066	PR	253.1539
AM	202.0776	EL	242.1267	HV	236.1273	PS	184.0848
AN	185.0801	EM	260.0831	HW	323.1382	PT	198.1004
AP	168.0899	EN	243.0855	HY	300.1223	PV	196.1212
AQ	199.0957	EP	226.0953	K	128.0950	PW	283.1321
AR	227.1382	EQ	257.1012	KK	256.1899	PY	260.1161
AS	158.0691	ER	285.1437	KL	241.1790	Q	128.0586
AT	172.0848	ES	216.0746	KM	259.1354	QQ	256.1172
AV	170.1055	ET	230.0903	KN	242.1379	QR	284.1597
AW	257.1164	EV	228.1110	KP	225.1477	QS	215.0906
AY	234.1004	EW	315.1219	KQ	256.1535	QT	229.1063
C	103.0092	EY	292.1059	KR	284.1960	QV	227.1270
CC	206.0184	F	147.0684	KS	215.1270	QW	314.1379
CD	218.0361	FF	294.1368	KT	229.1426	QY	291.1219
CE	232.0518	FG	204.0899	KV	227.1634	R	156.1011
CF	250.0776	FH	284.1273	KW	314.1743	RR	312.2022
CG	160.0307	FK	275.1634	KY	291.1583	RS	243.1331
CH	240.0681	FL	260.1525	L	113.0841	RT	257.1488
CK	231.1042	FM	278.1089	LL	226.1681	RV	255.1695
CL	216.0933	FN	261.1113	LM	244.1246	RW	342.1804
CM	234.0497	FP	244.1212	LN	227.1270	RY	319.1644
CN	217.0521	FQ	275.1270	LP	210.1368	S	87.0320
CP	200.0620	FR	303.1695	LQ	241.1426	SS	174.0641
CQ	231.0678	FS	234.1004	LR	269.1852	ST	188.0797
CR	259.1103	FT	248.1161	LS	200.1161	SV	186.1004
CS	190.0412	FV	246.1368	LT	214.1317	SW	273.1113
CT	204.0569	FW	333.1477	LV	212.1525	SY	250.0954
CV	202.0776	FY	310.1317	LW	299.1634	T	101.0477
CW	289.0885	G	57.0215	LY	276.1474	TT	202.0954
CY	266.0725	GG	114.0429	M	131.0405	TV	200.1161
D	115.0269	GH	194.0804	MM	262.0810	TW	287.1270
DD	230.0539	GK	185.1164	MN	245.0834	TY	264.1110
DE	244.0695	GL	170.1055	MP	228.0933	V	99.0684
DF	262.0953	GM	188.0620	MQ	259.0991	VV	198.1368
DG	172.0484	GN	171.0644	MR	287.1416	VW	285.1477
DH	252.0859	GP	154.0742	MS	218.0725	VY	262.1317
DK	243.1219	GQ	185.0801	MT	232.0882	W	186.0793
DL	228.1110	GR	213.1226	MV	230.1089	WW	372.1586
DM	246.0674	GS	144.0535	MW	317.1198	WY	349.1426
DN	229.0699	GT	158.0692	MY	294.1038	Y	163.0633
DP	212.0797	GV	156.0899	N	114.0429	YY	326.1267
DQ	243.0855	GW	243.1008	NN	228.0859		
DR	271.1281	GY	220.0848	NP	211.0957		
DS	202.0590	H	137.0589	NQ	242.1015		

*To calculate total mass of any two amino acid residues, first put the 2 single-letter codes in aphabelical order, then look them up in the table.

Reverse Mass Table*

Mass	Seq.	Mass	Seq.	Mass	Seq.	Mass	Seq.
16.0313	[CH_4]	199.0957	AQ, AAG	231.0855	GSS	256.1172	QQ, AAN, AQG
17.0265	[NH_3]	199.1321	AK	231.1042	CK	256.1535	QK, AGK
18.0106	[H_2O]	200.0620	CP	232.0518	CE	256.1899	KK
57.0215	G	200.0797	AE	232.0882	MT	257.0834	PC(+57), CGP
71.0371	A	200.1161	LS, TV	234.0497	CM	257.1012	EQ, AAD, AEG
87.0320	S	201.0750	NS, GGS	234.0674	SM(+16)	257.1164	AW
97.0528	P	202.0590	DS	234.1004	AY, FS	257.1376	EK, ASV, GLS GTV
99.0684	V	202.0776	AM, CV	234.1117	HP		
101.0477	T	202.0954	TT	236.1273	HV	257.1488	RT
103.0092	C	204.0569	CT, GM(+16)	238.0355	AS(+80), GT(+80)	258.0852	EE
113.0841	L	204.0899	GF	238.1066	HT	258.0964	NGS, GGGS
114.0429	N, GG	206.0184	CC	239.1270	AAP	259.0804	DGS
115.0269	D	208.0960	AH	240.0681	CH	259.0991	QM, VC(+57), AGM, CGV
128.0586	Q, AG	210.1368	LP	241.1063	GPS		
128.0950	K	211.0957	NP, GGP	241.1426	QL, AAV, AGL	259.1103	RC
129.0426	E	212.0797	DP	241.1790	LK	259.1168	AST, GTT
131.0405	M	212.1525	LV	242.1015	NQ, ANG, QGG, AGGG	259.1355	KM
137.0589	H	213.1113	NV, AAA, GGV			260.0831	EM
142.0742	AA	213.1226	RG	242.1266	EL	260.1161	PY
144.0535	GS	214.0954	DV	242.1379	NK, GGK	260.1195	LM(+16)
147.0354	M(+16)	214.1317	LT	243.0297	Y(+80)	260.1525	LF
147.0684	F	215.0906	NT, QS, AGS, GGT	243.0855	NE, DQ, ADG, EGG	261.0783	ACS, CGT, NM(+16), TC(+57), GGM(+16)
154.0742	GP						
156.0899	GV	215.1270	KS	243.1008	GW		
156.1011	R	216.0746	DT, ES	243.1219	DK, AAT, GSV	261.0961	SSS
158.0691	AS, GT	216.0933	CL	243.1331	RS	261.1113	NF, GGF
160.0307	C(+57), CG	217.0521	NC, GC(+57), CGG	244.0695	DE	262.0623	DM(+16)
163.0633	Y	218.0361	DC	244.0882	PM(+16)	262.0810	MM
166.9984	S(+80)	218.0725	AM(+16), MS	244.1212	FP	262.0954	DF
168.0899	AP	218.1055	AF	244.1246	LM	262.1317	YV
170.1055	AV, GL	220.0848	GY	245.0834	NM, AAC, GGM	263.0398	CC(+57), CCG
171.0644	NG, GGG	224.0198	GS(+80)	245.1012	ASS, GST	264.0511	PS(+80)
172.0484	DG	224.0909	HS	246.0674	DM	264.1110	TY
172.0848	AT	225.1113	QP, AGP	246.1038	VM(+16)	265.1175	QH, AGH
174.0463	AC	225.1477	KP	246.1368	FV	265.1426	APP
174.0641	SS	226.0954	EP	247.0627	SC(+57), CGS	265.1539	HK
181.0140	T(+80)	226.1681	LL	248.0831	TM(+16)	266.0668	VS(+80)
184.0848	PS	227.1270	NL, QV, AGV, GGL	248.1161	FT	266.0725	CY
184.1212	AL			250.0446	CM(+16)	266.1015	EH
185.0800	AN,QG,AGG	227.1382	AR	250.0776	CF	267.1583	APV, GLP
185.1164	GK	227.1634	KV	250.0954	SY	268.0460	ST(+80), TS(+80)
186.0640	EG	228.0858	GGGG	250.1430	HL	268.0994	HM
186.0641	AD	228.0859	NN, NGG	251.1018	NH, GGH	268.1171	GGGP
186.0793	W	228.0933	MP	251.1270	GPP	268.1172	NGP
186.1004	SV	228.1110	DL, EV	252.0511	AT(+80)	269.1012	DGP
188.0620	GM	229.0699	ND, DGG	252.0859	DH	269.1376	APT
188.0797	ST	229.1063	QT, AAS, AGT	253.1426	GPV	269.1739	AVV, GLV
190.0412	CS	229.1426	KT	253.1539	RP	269.1852	RL
194.0804	GH	230.0539	DD	254.0304	SS(+80)	270.0076	CS(+80)
194.1055	PP	230.0903	ET	255.1219	APS, GPT	270.1328	AAQ, NGV, AAAG, GGGV
196.1212	PV	230.1089	MV	255.1583	AAL, GVV		
198.1004	PT	231.0678	AC(+57), CQ, ACG	255.1695	RV	270.1440	RN, RGG
198.1368	VV			256.1171	AAGG	270.1692	AAK

* Three common PTMs are represented by their nominal mass in the sequence:
+57 - Carbamidomethyl (57.02146), +80 - Phosphorylation (79.96633), +16 - Oxidation on M (15.99491)

Common Amino Acid Residues

Name	3-letter Symbol	1-letter Symbol	Monoisotopic Mass	Average Mass	Residue Composition	Residue Structure
Alanine	Ala	A	71.03711	71.08	C_3H_5NO	CH_3 -NH-CH-CO-
Arginine	Arg	R	156.10111	156.2	$C_6H_{12}N_4O$	$-CH_2-(CH_2)_2-NH-C(=NH)-NH_2$ -NH-CH_2-CO-
Asparagine	Asn	N	114.04293	114.1	$C_4H_6N_2O_2$	CH_3-CONH_2 -NH-CH-CO-
Aspartic Acid	Asp	D	115.02694	115.1	$C_4H_5NO_3$	CH_3-COOH -NH-CH-CO-
Cysteine	Cys	C	103.00919	103.1	C_3H_5NOS	CH_2-SH -NH-CH-CO-
Glutamic Acid	Glu	E	129.04259	129.1	$C_5H_7NO_3$	CH_2-CH_2-COOH -NH-CH-CO-
Glutamine	Gln	Q	128.05858	128.1	$C_5H_8N_2O_2$	$CH_2-CH_2-CONH_2$ -NH-CH-CO-
Glycine	Gly	G	57.02146	57.05	C_2H_3NO	-NH-CH_2-CO-
Histidine	His	H	137.05891	137.1	$C_6H_7N_3O$	CH_2-(imidazole)- -NH-CH-CO-
Isoleucine	Ile	I	113.08406	113.2	$C_6H_{11}NO$	$CH(CH_3)-CH_2-CH_3$ -NH-CH-CO-
Leucine	Leu	L	113.08406	113.2	$C_6H_{11}NO$	$CH_2-CH(CH_3)_2$ -NH-CH-CO-
Lysine	Lys	K	128.09496	128.2	$C_6H_{12}N_2O$	$CH_2-(CH_2)_3-NH_2$ -NH-CH-CO-
Methionine	Met	M	131.04049	131.2	C_5H_9NOS	$CH_2-CH_2-S-CH_3$ -NH-CH-CO-
Phenyalanine	Phe	F	147.06841	147.2	C_9H_9NO	CH_2-(phenyl)- -NH-CH-CO-
Proline	Pro	P	97.05276	97.12	C_5H_7NO	-N-(cyclic)-CH-CO-
Serine	Ser	S	87.03203	87.08	$C_3H_5NO_2$	CH_2-OH -NH-CH-CO-
Threonine	Thr	T	101.04768	101.1	$C_4H_7NO_2$	$CH(OH)-CH_3$ -NH-CH-CO-
Tryptophan	Trp	W	186.07931	186.2	$C_{11}H_{10}N_2O$	$-CH_2$-(indole)- -NH-CH_2-CO-
Tyrosine	Tyr	Y	163.06333	163.2	$C_9H_9NO_2$	$-CH_2$-(phenyl)-OH -NH-CH_2-CO-
Valine	Val	V	99.06841	99.13	C_5H_9NO	$CH(CH_3)_2$ -NH-CH-CO-

Common PTMs

Monoisotopic Mass Δ	Position	Modification
-29.99281	[M]@C-term	Homoserine
-18.01057	Y, T, S, [N, Q]@C-term, [C]@N-term	Dehydration
-17.02655	[Q]@N-term	Pyroglutamic Acid from Gln
-2.01565	C	Disulphide Bond Formation
-0.98402	[X]@C-term	Amidation
0.98402	R	Citrullination
0.98402	R, N, Q	Deamidation
14.01565	T, S, E, D, L, I, [X]@N-term, R, Q, N, K, H, C, [X]@C-term	Methylation
15.99491	W, H, C, M	Oxidation
27.99491	T, K, S, [X]@N-term	Formylation (CHO)
42.01056	C, S, K, [X]@N-term	Acetylation
42.02180	K	Homoarginine
43.98983	W, K, D, E, [M]@N-term	Carboxylation
57.02146	C	Carbamidomethyl
58.00548	C	Carboxymethyl
79.96633	R, C, D, Y, H, T, S	Phosphorylation
79.95682	Y	Sulphation
119.00410	C	Cysteinylation
132.04226		Pentoses (Ara, Rib, Xyl)
146.05791		Deoxyhexoses (Fuc, Rha)
161.06881	K, N, T, W	Hexosamine (GalN, GlcN)
162.05282	Y, R, C, T, W, N, K, [X]@N-term	Hexoses (Fru, Gal, Glc, Man)
188.03296	K	Lipoic Acid (Amide Bond to Lys)
203.07937	S, T, N	N-acetylhexosamine (GalNAc, GlcNAc)
204.18780	C	Farnesylation
210.19836	K, C, [G]@N-term	Myristoylation
226.07760	K, [X]@N-term	Biotinylation (Amide Bond to Lys)
238.22966	C, K, S, T, [X]@N-term	Palmitoylation
272.25040	C	Geranylgeranylation
365.13220		Hex-HexNAc
541.06111	R, C, N, S, E	ADP-Ribosylation (from NAD)

Fragment Ions

Ion Type	Mass	Nominal Mass
a	[M] - 26.9871	[M] - 27
b	[M]+ 1.0078	[M]+1
c	[M]+ 18.0344	[M]+18
x	[M]+ 44.9977	[M]+ 45
y	[M]+ 19.0184	[M]+19
z	[M]+ 1.9918	[M]+ 2
z°	[M]+ 2.9997	[M]+ 3

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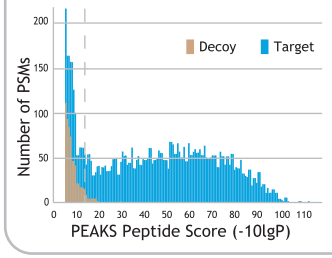
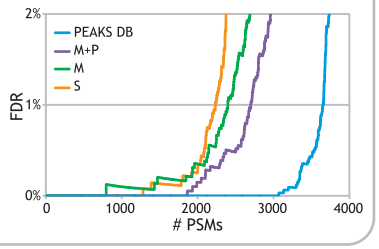
False Discovery Rate

A target protein DB is mixed with a decoy DB, and searched by peptide ID software. FDR = #decoy hits/#target hits. FDR is used to validate ID results (left fig.) and compare different software (right fig.)





Complete Analysis

A complete analysis tries to characterize every amino acid, including PTMs and mutations, of the protein. This offers advantages towards such applications as antibody sequencing, contaminant detection, and biomarker discovery. To achieve this, PEAKS integrates multiple algorithms for PTMs, mutations, novel peptides, and database peptides (left fig.); then visualizes all of them in a protein coverage view (right fig.).