Novabiochem®
Peptide Delta Masses

Amino-acid substitutions

-129.16	Trp to Gly
-115.13	Trp to Ala
-106.12	Tyr to Gly
-99.14	Arg to Gly
-99.13	Trp to Ser
-92.09	Tyr to Ala
-90.13	Phe to Gly
-89.09	Trp to Pro
-87.08	Trp to Val
-85.10	Trp to Thr
-85.11	Arg to Ala
-83.07	Trp to Cys
-80.09	His to Gly
-76.10	Phe to Ala
-76.09	Tyr to Ser
-74.15	Met to Gly
-73.05	Trp to Ile
-73.05	Trp to Leu
-72.11	Trp to Asn
-72.07	Glu to Gly
-71.12	Trp to Asp
-71.12	Lys to Gly
-71.08	Gln to Gly
-69.11	Arg to Ser
-66.06	His to Ala
-66.05	Tyr to Pro
-64.04	Tyr to Val
-62.06	Tyr to Thr
-60.12	Met to Ala
-60.10	Phe to Ser
-60.03	Tyr to Cys
-59.07	Arg to Pro
-58.08	Trp to Gln
-58.04	Trp to Lys
-58.04	Asp to Gly
-58.04	Glu to Ala
-57.09	Trp to Glu
-57.09	Lys to Ala
-57.06	Arg to Val
-57.05	Gln to Ala
-57.05	Asn to Gly
-56.11	Ile to Gly
-56.11	Leu to Gly
-55.08	Arg to Thr
-55.01	Trp to Met
-53.05	Arg to Cys
-50.06	Phe to Pro
-50.06	His to Ser
-50.01	Tyr to Ile
-50.01	Tyr to Leu
-49.07	Trp to His
-49.07	Tyr to Asn
-48.08	Tyr to Asp
-48.05	Phe to Val
-46.09	Cys to Gly
-46.07	Phe to Thr
-44.12	Met to Ser
-44.06	Thr to Gly
-44.04	Phe to Cys
-44.01	Asp to Ala
-43.03	Arg to Ile
-43.03	Arg to Leu
-43.02	Asn to Ala
-42.09	Arg to Asn
-42.08	Leu to Ala
-42.08	Ile to Ala
-42.08	Val to Gly
-42.04	Glu to Ser
-41.10	Arg to Asp
-41.09	Lys to Ser
-41.05	Gln to Ser
-40.07	Pro to Gly
-40.02	His to Pro
-39.03	Trp to Phe
-38.01	His to Val
-36.03	His to Thr
-35.04	Tyr to Gln
-35.00	Tyr to Lys
-34.08	Met to Pro
-34.05	Tyr to Glu
-34.02	Phe to Ile
-34.02	Phe to Leu
-34.02	Phe to Lys
-34.00	His to Cys
-33.08	Phe to Asn
-32.09	Phe to Asp
-32.07	Met to Val
-32.06	Cys to Ala
-32.00	Glu to Pro
-31.97	Tyr to Met
-31.05	Lys to Pro
-31.01	Gln to Pro
-30.09	Met to Thr
-30.03	Ser to Gly
-30.03	Thr to Ala
-30.02	Trp to Arg
-29.99	Glu to Val
-29.04	Lys to Val
-29.00	Gln to Val
-28.06	Arg to Gln
-28.06	Met to Cys
-28.05	Val to Ala
-28.02	Arg to Lys
-28.01	Glu to Thr
-28.01	Asp to Ser
-27.07	Arg to Glu
-27.06	Lys to Thr
-27.02	Gln to Thr
-27.02	Asn to Ser
-26.08	Ile to Ser
-26.08	Leu to Ser
-26.04	Pro to Ala
-26.03	Tyr to His
-25.98	Glu to Cys
-25.03	Lys to Cys
-24.99	Arg to Met
-24.99	Gln to Cys
-23.98	His to Ile
-23.98	His to Leu
-23.04	His to Asn
-23.04	Trp to Tyr
-22.05	His to Asp
-19.05	Arg to His
-19.05	Phe to Gln
-19.01	Phe to Lys
-18.06	Phe to Glu
-18.04	Met to Ile
-18.04	Met to Leu
-17.97	Asp to Pro
-17.10	Met to Asn
-16.98	Asn to Pro
-16.11	Met to Asp
-16.06	Cys to Ser
-16.04	Ile to Pro
-16.04	Leu to Pro
-16.00	Ser to Ala
-15.99	Tyr to Phe
-15.98	Phe to Met
-15.96	Asp to Val
-15.96	Glu to Ile
-15.96	Glu to Leu
-15.02	Glu to Asn
-15.01	Lys to Ile
-15.01	Lys to Leu
-14.97	Gln to Ile
-14.97	Gln to Leu
-14.97	Asn to Val
-14.07	Lys to Asn
-14.03	Gln to Asn
-14.03	Ile to Val
-14.03	Leu to Val
-14.03	Ala to Gly
-14.03	Glu to Asp
-14.03	Thr to Ser
-13.98	Asp to Thr
-13.08	Lys to Asp
-13.04	Gln to Asp
-12.99	Asn to Thr
-12.06	Ile to Thr
-12.05	Leu to Thr
-12.05	Val to Ser
-11.95	Asp to Cys
-10.96	Asn to Cys
-10.04	Phe to His
-10.04	Pro to Ser
-10.02	Ile to Cys
-10.02	Leu to Cys
-9.01	Arg to Phe
-9.01	His to Gln
-8.97	His to Lys
-8.02	His to Glu
-6.98	Tyr to Arg
-6.02	Cys to Pro
-5.94	His to Met
-4.01	Cys to Val
-3.99	Thr to Pro
-3.07	Met to Gln
-3.03	Met to Lys
-2.08	Met to Glu
-2.03	Cys to Thr
-2.01	Val to Pro
-1.98	Thr to Val
-1.93	Asp to Ile
-1.93	Asp to Leu
-0.99	Asp to Asn
-0.99	Glu to Gln
-0.95	Glu to Lys
-0.94	Asn to Ile
-0.94	Asn to Leu
-0.04	Lys to Gln

Single amino-acid and dipeptide deletions

-372	TrpTrp
-349	TrpTyr
-342	ArgTrp
-333	PheTrp
-326	TyrTyr
-323	HisTrp
-319	ArgTyr
-317	MetTrp
-315	GluTrp
-314	GlnTrp
-314	LysTrp
-312	ArgArg
-310	PheTyr
-303	ArgPhe
-301	AspTrp
-300	AsnTrp
-300	HisTyr
-299	IleTrp
-299	LeuTrp
-294	MetTyr
-294	PhePhe
-293	ArgHis
-292	GluTyr
-291	GlnTyr
-291	LysTyr
-289	CysTrp
-287	ArgMet
-287	ThrTrp
-285	ArgGlu
-285	TrpVal
-284	ArgGln
-284	ArgLys
-284	HisPhe
-283	ProTrp
-278	AspTyr
-278	MetPhe
-277	AsnTyr
-276	GluPhe
-276	IleTyr
-276	LeuTyr
-275	GlnPhe
-275	LysPhe
-274	HisHis
-273	SerTrp
-271	ArgAsp
-270	ArgAsn
-269	ArgIle
-269	ArgLeu
-268	HisMet
-266	CysTyr
-266	GluHis
-265	GlnHis
-265	HisLys
-264	ThrTyr
-262	AspPhe
-262	MetMet
-262	TyrVal
-261	AsnPhe
-260	GluMet
-260	IlePhe
-260	LeuPhe
-260	ProTyr
-259	ArgCys
-259	GlnMet
-259	LysMet
-258	GluGlu
-257	AlaTrp
-257	ArgThr
-257	GlnGlu
-257	GluLys
-256	GlnGln
-256	GlnLys
-256	LysLys
-255	ArgVal
-253	ArgPro
-252	AspHis
-251	AsnHis
-250	CysPhe
-250	HisIle
-250	HisLeu
-250	SerTyr
-248	PheThr
-246	AspMet
-246	PheVal
-245	AsnMet
-244	AspGlu
-244	IleMet
-244	LeuMet
-244	PhePro
-243	pTyr
-243	Tyr(SO$_3$H)
-243	ArgSer
-243	AsnGlu
-243	AspGln
-243	AspLys
-243	GlyTrp
-242	AsnGln
-242	AsnLys
-242	GluIle
-242	GluLeu
-241	GlnIle
-241	GlnLeu
-241	IleLys
-241	LeuLys
-240	CysHis
-238	HisThr
-236	HisVal
-234	AlaTyr
-234	CysMet
-234	HisPro
-234	PheSer
-232	CysGlu
-232	MetThr
-231	CysGln
-231	CysLys
-230	AspAsp
-230	GluThr
-230	MetVal
-229	AsnAsp
-229	GlnThr
-229	LysThr
-228	AsnAsn
-228	AspIle
-228	AspLeu
-228	GluVal
-228	MetPro
-227	AlaArg
-227	AsnIle
-227	AsnLeu
-227	GlnVal
-227	LysVal
-226	GluPro
-226	IleIle
-226	IleLeu
-226	LeuLeu
-225	GlnPro
-225	LysPro
-224	HisSer
-220	GlyTyr
-218	AlaPhe
-218	AspCys
-218	MetSer
-217	AsnCys
-216	AspThr
-216	CysIle
-216	CysLeu
-216	GluSer
-215	AsnThr
-215	GlnSer
-215	LysSer
-214	AspVal
-214	IleThr
-214	LeuThr
-213	ArgGly
-213	AsnVal
-212	AspPro
-212	IleVal
-212	LeuVal
-211	AsnPro
-210	IlePro
-210	LeuPro
-208	AlaHis
-206	CysCys
-204	CysThr
-204	GlyPhe
-202	AlaMet
-202	AspSer
-202	CysVal
-202	ThrThr
-201	AsnSer
-200	AlaGlu
-200	CysPro
-200	IleSer
-200	LeuSer
-200	ThrVal
-199	AlaGln
-199	AlaLys
-198	ProThr
-198	ValVal
-196	ProVal
-194	GlyHis
-194	ProPro
-190	CysSer
-188	GlyMet
-188	SerThr
-186	Trp
-186	AlaAsp
-186	GluGly
-186	SerVal
-185	AlaAsn
-185	GlnGly
-185	GlyLys
-184	Arg(Me$_2$)
-184	AlaIle
-184	AlaLeu
-184	ProSer
-181	pThr
-174	AlaCys
-174	SerSer
-172	AlaThr
-172	AspGly
-171	AsnGly
-171	Lys(Me$_2$)
-170	Arg(Me)
-170	AlaVal
-170	GlyIle
-170	GlyLeu
-168	AlaPro
-167	pSer
-163	Tyr
-160	CysGly
-158	AlaSer
-158	GlyThr
-157	Cit
-156	Arg
-156	GlyVal
-156	Lys(Me$_2$)
-154	GlyPro
-153	Cha
-147	Phe
-144	GlySer
-142	Lys(Me)
-142	AlaAla
-137	His
-131	Met
-129	Glu
-128	Gln, Lys
-128	AlaGly
-115	Asp
-114	Asn, Orn
-114	GlyGly
-113	Ile, Leu, Hyp, Nle, ε-Ahx
-103	Cys
-101	hSer, Thr
-99	Val
-97	Pro
-95	dPro
-87	Ser
-85	Abu, γ-Abu, Aib
-71	Ala, β-Ala, Sar
-57	Gly

Adducts, modifications, and protecting groups

-98	H_3PO_4; artifact observed during MS of pSer and pThr peptides
-80	Dephosphorylation: avoid prolonged storage of phosphopeptides in acid aqueous media
-42	Orn formation from Arg
-34	Dehydroalanine from Cys
-32	Lanthionine formation from cystine
-18	Pyr formation from Glu; avoid using benzyl or allyl protection for N-terminal Glu residues
-18	Dehydration (-H_2O)
-18	Ser to dehydroalanine
-18	Cyanoalanine formation from Asn; use side-chain protected Asn derivatives
-18	Aspartimide formation from Asp; use Fmoc-Asp(OtBu)-(Dmb)Gly-OH or Fmoc-Asp(OMpe)-OH
-18	Pyrophosphate formation with peptide containing 2 adjacent phosphoresidues
-17	Pyr formed from Gln; avoid N-terminal Gln residues
-17	Aspartimide formation from Asn
-16	H-Phosphonate formation if a phosphopeptide; use benzyl protected phosphoramidites and anhydrous t-butyl hydroperoxide for oxidation
-13	N-Piperidinylalanine formation from pSer or pThr; avoid using microwave heating for Fmoc removal
-2	Disulfide bond formation from cystine
-1	Amide formation (C terminus)
1	Deamidation of Asn and Gln to Asp and Glu; avoid leaving peptide in aqueous media for prolonged periods
1	Cit formation from Arg
2	Reduction of cystine
2	Reduction of indole double bond of Trp; use Trp(Boc) and avoid use of TES
12	Cys to thioproline conversion, due to formaldehyde contamination of acetic acid
12	Formaldehyde adduct of Trp
14	Methyl ester; ensure peptide resin is free from methanol before cleavage
14	Hydrazide formation from free acid
16	Oxidation of Met to sulfoxide
16	Sulfenic Acid from Cys
17	Ammonium adduct
22	Sodium adduct
28	Ethyl
28	Formyl; use good quality DMF and avoid heating peptides dissolved in formic acid
32	Oxidation of Met to sulfone
38	Potassium adduct
40	Uncleaved pseudoproline; extend cleavage and add EDT
41	MeCN adduct of Lys
42	Ac
44	Disodium adduct
44	CO_2 adduct of Trp; dissolve in 1% AcOH aq. and freeze dry.
45	Nitro
48	Cysteic acid formation by oxidation of Cys
51	β-Piperidinylalanine formation from C-terminal Cys; use trityl resin such as 2-chlorotrityl chloride resin or NovaSyn TGT
56	tBu; alkylation adduct of Cys, Met, Trp, Tyr
57	Gly insertion; avoid Gly symmetrical anhydride
60	Sodium-potassium adduct
67	Asp piperidide formation; use Fmoc-Asp(OtBu)-(Dmb)Gly-OH or Fmoc-Asp(OMpe)-OH
71	Acm
76	Mercaptoethanol adduct
80	Sulfonation (SO_3H) (Arg, Ser, Thr from Pbf or Pmc); recleave with TMSBr/thioanisole/EDT/TFA.
80	Sulfation of Tyr
80	Phosphorylation
82	cHex
82	Dmcp
84	Mpe
86	Bum
88	StBu
90	Bzl; uncleaved phosphoamino acid protecting group or alkyation adduct of Cys, Trp or Tyr.
91	Bzl alkyation of Met.
92	EDT disulfide adduct; reduce with TCEP
96	Tfa; treat peptide with 0.1 M ammonium bicarbonate to cleave Tfa esters
97	Pro insertion; avoid double coupling of Pro
98	Tetramethylguanidinium termination by-product on amine; use phosphonium reagents instead of uronium
100	Boc
104	MeBzl
104	Bz
106	HMP adduct; use an HMPA resin, such as NovaSyn TGA instead of a Wang resin, or Rink Amide AM resin instead of Rink Amide resin
111	Pyr insertion; use Pyr-OPcp for Pyr introduction
117	Succinyl
118	PhiPr
120	MeOBzl
134	Z
134	Ada
136	Hmb
150	Dmb
152	DDT disulfide adduct
153	Nps
154	Tos
154	Npys
163	Methylphenoxyacetamide - adduct of Knorr linker; use Rink Amide AM resin instead of Rink Amide MBHA resin
166	Dnp
172	Ethanedithiol/TFA cyclic adduct; Use Trp(Boc) instead of Trp and avoid pro-longed cleavage times when EDT is used as scavenger
178	AcHmb
180	Tmob
180	Xan
182	Mts
188	Alkylation of Trp by Pbf chroman
189	α-Cyanocinnapinic acid adduct
201	HMP (hydroxymethylphenyl)/TFA adduct
204	S-Farnesyl
206	ivDde
212	Mtr
216	Mca
222	Fmoc
226	Biotinyl
226	Mbh
233	Dansyl
238	Bpoc
238	Palmitoylation
242	Trt
243	Rink amide linker adduct; use Rink Amide AM resin.
251	Dabcyl
252	Pbf
256	Mtt
264	EDANS
266	Stearoylation
266	Pmc
268	Biotinyl-aminoethylamino (from Biotin NovaTag) addition to mass of peptide acid
272	Mmt
299	Knorr linker adduct; use Rink Amide AM resin instead of Rink Amide MBHA
304	Glutathione disulfide adduct
312	Dmab
358	FAM
412	TAMRA
428	Biotinyl-PEG (from Biotin PEG NovaTag resin addition to mass of peptide acid

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