PTM (AA)	chemical	MW (u)	SASA (nm^2)	net charge	DM (D)
S1P (SER)	phosphoserine (-1)	110.0 (31.0)	1.88 (1.20)	-1 (0)	N/A (2.30)
S2P (SER)	phosphoserine (-2)	109.0 (31.0)	1.93 (1.20)	-2 (0)	N/A (2.30)
T1P (THR)	phosphothreonine (-1)	124.0 (45.1)	2.12 (1.41)	-1 (0)	N/A (2.23)
T2P (THR)	phosphothreonine (-2)	123.0 (45.1)	2.15 (1.41)	-2 (0)	N/A (2.23)
Y1P (TYR)	phosphotyrosine (-1)	186.1 (107.1)	2.81 (2.41)	-1 (0)	N/A (2.06)
Y2P (TYR)	phosphotyrosine (-2)	185.1 (107.1)	2.73 (2.41)	-2 (0)	N/A (2.06)
D1P (ASP)	phosphoaspartate (-1)	138.0 (58.0)	2.23 (1.57)	-1 (-1)	N/A (N/A)
D2P (ASP)	phosphoaspartate (-2)	137.0 (58.0)	2.17 (1.57)	-2 (-1)	N/A (N/A)
K1P (LYS)	phospholysine (-1)	151.1 (73.1)	2.59 (1.92)	-1 (1)	N/A (N/A)
K2P (LYS)	phospholysine (-2)	150.1 (73.1)	2.54 (1.92)	-2 (1)	N/A (N/A)
R0P (ARG)	phosphoarginine (0)	180.1 (101.2)	2.82 (2.21)	0 (1)	14.65 (N/A)
R1P (ARG)	phosphoarginine (-1)	179.1 (101.2)	2.73 (2.21)	-1 (1)	N/A (N/A)
H11 (HIS)	1-phosphohistidine (-1)	160.1 (81.1)	2.36 (1.91)	-1 (0)	N/A (6.43)
H12 (HIS)	1-phosphohistidine (-2)	159.1 (81.1)	2.39 (1.91)	-2 (0)	N/A (6.43)
H31 (HIS)	3-phosphohistidine (-1)	160.1 (81.1)	2.51 (1.91)	-1 (0)	N/A (6.43)
H32 (HIS)	3-phosphohistidine (-2)	159.1 (81.1)	2.53 (1.91)	-2 (0)	N/A (6.43)
KMN (LYS)	N6-methyllysine (0)	86.2 (73.1)	2.40 (1.92)	0 (1)	1.84 (N/A)
KMC (LYS)	N6-methyllysine (+1)	87.2 (73.1)	2.26 (1.92)	1 (1)	N/A (N/A)
K2M (LYS)	N6,N6-dimethyllysine (0)	100.2 (73.1)	2.72 (1.92)	0 (1)	1.58 (N/A)
K2C (LYS)	N6,N6-dimethyllysine (+1)	101.2 (73.1)	2.45 (1.92)	1 (1)	N/A (N/A)
K3C (LYS)	N6,N6,N6-trimethyllysine	115.2 (73.1)	2.68 (1.92)	1 (1)	N/A (N/A)
RMN (ARG)	omega-N-methylarginine (0)	114.2 (101.2)	2.38 (2.21)	0 (1)	2.78 (N/A)
RMC (ARG)	omega-N-methylarginine (+1)	115.2 (101.2)	2.43 (2.21)	1 (1)	N/A (N/A)
RSM (ARG)	symmetric-dimethylarginine (0)	128.2 (101.2)	2.80 (2.21)	0 (1)	0.94 (N/A)
RMS (ARG)	symmetric-dimethylarginine (+1)	129.2 (101.2)	2.69 (2.21)	1 (1)	N/A (N/A)

RAM (ARG)	asymmetric-dimethylarginine (0)	128.2 (101.2)	2.62 (2.21)	0 (1)	3.55 (N/A)
RMA (ARG)	asymmetric-dimethylarginine (+1)	129.2 (101.2)	2.69 (2.21)	1 (1)	N/A (N/A)
H1M (HIS)	1-methylhistidine (0)	95.1 (81.1)	2.24 (1.91)	0 (0)	6.10 (6.43)
H1C (HIS)	1-methylhistidine (+1)	96.1 (81.1)	2.19 (1.91)	1 (0)	N/A (6.43)
H3M (HIS)	3-methylhistidine (0)	95.1 (81.1)	2.32 (1.91)	0 (0)	4.33 (6.43)
H3C (HIS)	3-methylhistidine (+1)	96.1 (81.1)	2.01 (1.91)	1 (0)	N/A (6.43)
QME (GLN)	N5-methylglutamine	86.1 (72.1)	2.07 (1.80)	0 (0)	2.28 (4.94)
NME (ASN)	N4-methylasparagine	72.1 (58.1)	1.97 (1.56)	0 (0)	4.14 (4.90)
EME (GLU)	glutamate methyl ester	87.1 (72.1)	1.99 (1.79)	0 (-1)	5.27 (N/A)
DMA (ASP)	aspartate methyl ester	73.1 (58.0)	1.80 (1.57)	0 (-1)	5.31 (N/A)
CYM (CYS)	S-methylcysteine	61.1 (47.1)	1.65 (1.41)	0 (0)	2.74 (1.84)
KAC (LYS)	N6-acetyllysine	114.2 (73.1)	2.67 (1.92)	0 (1)	4.12 (N/A)
PH3 (PRO)	3-hydroxyproline (R)	58.1 (42.1)	1.61 (1.59)	0 (0)	2.32 (N/A)
P3H (PRO)	3-hydroxyproline (S)	58.1 (42.1)	1.64 (1.59)	0 (0)	2.27 (N/A)
HYP (PRO)	4-hydroxyproline (R)	58.1 (42.1)	1.77 (1.59)	0 (0)	2.14 (N/A)
HY2 (PRO)	4-hydroxyproline (S)	58.1 (42.1)	1.67 (1.59)	0 (0)	2.20 (N/A)
PHH (PRO)	3,4-dihydroxyproline	74.1 (42.1)	1.76 (1.59)	0 (0)	3.66 (N/A)
KH5 (LYS)	5-hydroxylysine (0,R)	88.1 (73.1)	2.03 (1.92)	0 (1)	3.62 (N/A)
K5H (LYS)	5-hydroxylysine (0,S)	88.1 (73.1)	2.17 (1.92)	0 (1)	5.86 (N/A)
KPH (LYS)	5-hydroxylysine (+1,R)	89.1 (73.1)	2.05 (1.92)	1 (1)	N/A (N/A)
KHP (LYS)	5-hydroxylysine (+1,S)	89.1 (73.1)	2.03 (1.92)	1 (1)	N/A (N/A)
HTY (TYR)	3,4-dihydroxyphenylalanine	123.1 (107.1)	2.29 (2.41)	0 (0)	3.97 (2.06)
W7H (TRP)	7-hydroxytryptophan	146.2 (130.2)	2.70 (2.63)	0 (0)	3.19 (3.65)
DH3 (ASP)	3-hydroxyaspartate (-1,R)	74.0 (58.0)	1.52 (1.57)	-1 (-1)	N/A (N/A)
D3H (ASP)	3-hydroxyaspartate (-1,S)	74.0 (58.0)	1.57 (1.57)	-1 (-1)	N/A (N/A)
DN3 (ASP)	3-hydroxyaspartate (0,R)	75.0 (58.0)	1.61 (1.57)	0 (-1)	0.58 (N/A)

D3N (ASP)	3-hydroxyaspartate (0,S)	75.0 (58.0)	1.56 (1.57)	0 (-1)	3.79 (N/A)
N3H (ASN)	3-hydroxyasparagine (R)	74.1 (58.1)	1.71 (1.56)	0 (0)	3.34 (4.90)
NH3 (ASN)	3-hydroxyasparagine (S)	74.1 (58.1)	1.84 (1.56)	0 (0)	6.30 (4.90)
ECA (GLU)	4-carboxyglutamate (-2)	115.1 (72.1)	2.06 (1.79)	-2 (-1)	N/A (N/A)
ECN (GLU)	4-carboxyglutamate (-1)	116.1 (72.1)	2.20 (1.79)	-1 (-1)	N/A (N/A)
YSU (TYR)	sulfotyrosine	186.2 (107.1)	2.66 (2.41)	-1 (0)	N/A (2.06)
SDH (SER)	dehydroalanine	14.0 (31.0)	1.06 (1.20)	0 (0)	0.00 (2.30)
TDH (THR)	2,3-didehydrobutyrine	28.1 (45.1)	1.39 (1.41)	0 (0)	0.00 (2.23)
WBR (TRP)	6-bromotryptophan	209.1 (130.2)	2.88 (2.63)	0 (0)	3.16 (3.65)
CSN (CYS)	S-nitrosocysteine	76.1 (47.1)	1.71 (1.41)	0 (0)	3.15 (1.84)
RCI (ARG)	citrulline	101.1 (101.2)	2.22 (2.21)	0 (1)	5.21 (N/A)
KAL (LYS)	allysine (aminoadipic semialdehyde)	71.1 (73.1)	2.04 (1.92)	0 (1)	2.96 (N/A)
NNG (ASN)	N-acetylglucosamine	261.3 (58.1)	3.73 (1.56)	0 (0)	9.10 (4.90)
F23 (PHE)	2,3-dihydroxyphenylalanine	123.1 (91.1)	2.29 (2.28)	0 (0)	4.55 (0.74)
F2H (PHE)	2-hydroxyphenylalanine	107.1 (91.1)	2.13 (2.28)	0 (0)	3.11 (0.74)
F3H (PHE)	3-hydroxyphenylalanine	107.1 (91.1)	2.08 (2.28)	0 (0)	2.73 (0.74)
TYR (PHE)	tyrosine	107.1 (91.1)	2.41 (2.28)	0 (0)	2.06 (0.74)
W6H (TRP)	6-hydroxytryptophan	146.2 (130.2)	2.75 (2.63)	0 (0)	1.32 (3.65)
W5H (TRP)	5-hydroxytryptophan	146.2 (130.2)	2.71 (2.63)	0 (0)	3.46 (3.65)
W4H (TRP)	4-hydroxytryptophan	146.2 (130.2)	2.71 (2.63)	0 (0)	4.88 (3.65)
W2H (TRP)	2-hydroxytryptophan	146.2 (130.2)	2.73 (2.63)	0 (0)	5.19 (3.65)
L3H (LEU)	3-hydroxyleucine (R)	73.1 (57.1)	1.96 (1.88)	0 (0)	2.23 (0.00)
LH3 (LEU)	3-hydroxyleucine (S)	73.1 (57.1)	1.86 (1.88)	0 (0)	2.25 (0.00)
L4H (LEU)	4-hydroxyleucine	73.1 (57.1)	1.92 (1.88)	0 (0)	2.19 (0.00)
L5H (LEU)	5-hydroxyleucine (R)	73.1 (57.1)	1.98 (1.88)	0 (0)	2.17 (0.00)
LH5 (LEU)	5-hydroxyleucine (S)	73.1 (57.1)	2.01 (1.88)	0 (0)	2.19 (0.00)

V3H (VAL)	3-hyroxyvaline	59.1 (43.1)	1.70 (1.55)	0 (0)	2.30 (0.00)
CYH (CYS)	cysteine sulfenic acid	63.1 (47.1)	1.62 (1.41)	0 (0)	2.38 (1.84)
PH5 (PRO)	5-hydroxyproline (R)	58.1 (42.1)	1.69 (1.59)	0 (0)	2.21 (N/A)
P5H (PRO)	5-hydroxyproline (S)	58.1 (42.1)	1.79 (1.59)	0 (0)	2.17 (N/A)
GSA (PRO)	glutamic semialdehyde	57.1 (42.1)	1.64 (1.59)	0 (0)	2.95 (N/A)
GSA (ARG)	glutamic semialdehyde	57.1 (101.2)	1.64 (2.21)	0 (1)	2.95 (N/A)
TOX (THR)	2-amino-3-ketobutyric acid	43.0 (45.1)	1.40 (1.41)	0 (0)	2.66 (2.23)
PGA (PRO)	pyroglutamic acid	56.1 (42.1)	1.74 (1.59)	0 (0)	2.65 (N/A)
ASN (HIS)	asparagine	58.1 (81.1)	1.56 (1.91)	0 (0)	4.90 (6.43)
ASP (HIS)	aspartic acid (-1)	58.0 (81.1)	1.57 (1.91)	-1 (0)	N/A (6.43)
H2X (HIS)	2-oxo-histidine	95.1 (81.1)	2.00 (1.91)	0 (0)	9.64 (6.43)
MSX (MET)	methionine sulfoxide (R)	91.2 (75.2)	2.02 (1.94)	0 (0)	4.27 (2.62)
MXS (MET)	methionine sulfoxide (S)	91.2 (75.2)	2.11 (1.94)	0 (0)	4.23 (2.62)
MES (MET)	methionine sulfone	107.2 (75.2)	2.14 (1.94)	0 (0)	6.80 (2.62)
CSA (CYS)	cysteine sulfinic acid	78.1 (47.1)	1.69 (1.41)	-1 (0)	N/A (1.84)
CSE (CYS)	cysteic acid	94.1 (47.1)	1.80 (1.41)	-1 (0)	N/A (1.84)
YNI (TYR)	3-nitrotyrosine (-1)	151.1 (107.1)	2.61 (2.41)	-1 (0)	N/A (2.06)
YNN (TYR)	3-nitrotyrosine (0)	152.1 (107.1)	2.62 (2.41)	0 (0)	5.44 (2.06)
YNB (TYR)	3-nitrotyrosine (0)	152.1 (107.1)	2.62 (2.41)	0 (0)	3.83 (2.06)
WNI (TRP)	6-nitrotryptophan	175.2 (130.2)	3.06 (2.63)	0 (0)	3.08 (3.65)
WKY (TRP)	kynurenine	134.2 (130.2)	2.60 (2.63)	0 (0)	4.16 (3.65)
WKH (TRP)	3-hydroxykynurenine	150.2 (130.2)	2.66 (2.63)	0 (0)	2.78 (3.65)
WKF (TRP)	formylkynurenine	162.2 (130.2)	2.98 (2.63)	0 (0)	3.03 (3.65)
YCH (TYR)	chlorotyrosine	141.6 (107.1)	2.44 (2.41)	0 (0)	3.43 (2.06)
ASP (ASN)	aspartic acid (-1)	58.0 (58.1)	1.57 (1.56)	-1 (0)	N/A (4.90)
GLU (GLN)	glutamic acid (-1)	72.1 (72.1)	1.79 (1.80)	-1 (0)	N/A (4.94)

KAM (LYS)	homocitruline	115.2 (73.1)	2.46 (1.92)	0 (1)	5.24 (N/A)
KCA (LYS)	carboxylysine (+1)	115.1 (73.1)	2.48 (1.92)	-1 (1)	N/A (N/A)
KCN (LYS)	carboxylysine (0)	116.1 (73.1)	2.49 (1.92)	0 (1)	3.63 (N/A)
CAM (CYS)	S-carbamoylcysteine	90.1 (47.1)	1.99 (1.41)	0 (0)	4.81 (1.84)
LNO (LEU)	norleucine	57.1 (57.1)	1.88 (1.88)	0 (0)	0.00 (0.00)
LNO (LYS)	norleucine	57.1 (73.1)	1.88 (1.92)	0 (1)	0.00 (N/A)
LNO (MET)	norleucine	57.1 (75.2)	1.88 (1.94)	0 (0)	0.00 (2.62)