

t-Butyldimethylsilyl (tBDMS)-Derivative / EI Ionization															
											M=AA+2*tBDMS				
											2*tBDMS=	228.15			
		Composition							MW	Add deriv units:					
	atom:	C	H	O	N	S		(AA)	tBDMS-	tBDMS-	[M] ⁺	[M-tB] ⁺	[M-COOtBDMS] ⁺	[M-CoTB] ⁺	
Species	mass:	12	1	16	14	32			on COOH	on NH2, OH, SH					
	defect:	0	0.007	-0.005	0.003	-0.028			114.07	114.07	0.00	-57.06	-159.07	-85.06	
Alanine		3	7	2	1			89.04			317.19	260.13	158.12	232.13	
Arginine		6	14	2	4			174.10		2	630.40	573.33	471.33	545.34	
Asparagine		4	8	3	2			132.05	1		474.27	417.21	315.20	389.21	
Aspartate		4	7	4	1			133.03	1		475.25	418.19	316.18	390.20	
Cysteine		3	7	2	1	1		121.01		1	463.24	406.17	304.17	378.18	
DABA		4	10	2	2			118.07		2	574.36	517.30	415.29	489.30	
Glutamate		5	9	4	1			147.05	1		489.27	432.20	330.20	404.21	
Glutamine		5	10	3	2			146.06		1	488.28	431.22	329.21	403.22	
Glycine		2	5	2	1			75.03			303.18	246.11	144.11	218.12	
Histidine		6	9	2	3			155.06		1	497.28	440.22	338.21	412.23	
Isoleucine		6	13	2	1			131.08			359.23	302.17	200.16	274.17	
Leucine		6	13	2	1			131.08			359.23	302.17	200.16	274.17	
Lysine		6	14	2	2			146.09		1	488.32	431.25	329.25	403.26	
Me.Histidine		7	11	2	3			169.08			397.22	340.16	238.15	312.17	
Methionine		5	11	2	1	1		149.04			377.19	320.13	218.12	292.13	
OH-Lysine		6	14	3	2			162.09		2	618.38	561.32	459.31	533.33	
OH-Proline		5	9	3	1			131.05		1	473.27	416.21	314.20	388.21	
Ornithine		5	12	2	2			132.08		1	474.30	417.24	315.23	389.24	
Phenylalanine		9	11	2	1			165.07			393.22	336.15	234.15	308.16	
Proline (2)		5	9	2	1			115.06			343.20	286.14	184.13	258.15	
Pyroglutamate (1)		5	7	3	1			129.04		-1	243.11	186.05	84.04	158.05	
Pyroglutamate (2)		5	7	3	1			129.04			357.18	300.12	198.11	272.13	
Serine		3	7	3	1			105.04		1	447.26	390.20	288.19	362.20	
Theanine (2)		7	14	3	2			174.09			402.24	345.17	243.17	317.18	
Theanine (3)		7	14	3	2			174.09		1	516.31	459.25	357.24	431.25	
Threonine		4	9	3	1			119.05		1	461.27	404.21	302.20	376.21	
Tryptophan		11	12	2	2			204.08			432.23	375.16	273.16	347.17	
Tyrosine		9	11	3	1			181.06		1	523.29	466.22	364.22	438.23	
Valine		5	11	2	1			117.07			345.22	288.15	186.15	260.16	
Urea		1	4	1	2			60.03	-1	1	288.18	231.11	129.11	203.12	
KIC		6	10	3				130.05			259.11	o-phenylenediamine			
KIV		5	8	3				116.04			245.10	tBDMS			
KC		6	10	3				130.05			259.11	for KIC, KIV KC			
DABA = 2,4-diaminobutyrate															

Heptafluorobutyryl <i>n</i> -Propyl (HFBP) Derivative / EI Ionization												
											M=AA+HFB+Pr	
											HFB+Pr=	238.02
		Composition						MW	Add deriv units:			
	atom:	C	H	O	N	S		(AA)	Propyl-	HFB-	[M-COOPr] ⁺	
Species	mass:	12	1	16	14	32			on COOH	on NH2, OH, SH		
	defect:	0	0.007	-0.005	0.003	-0.028			42.04	195.97	-87.04	
Alanine		3	7	2	1			89.04			240.02	
Arginine		6	14	2	4			174.10		2	717.02	
Asparagine		4	8	3	2			132.05	1		325.07	
Aspartate		4	7	4	1			133.03	1		326.05	
Cysteine		3	7	2	1	1		121.01		1	467.96	
DABA												
Glutamate		5	9	4	1			147.05	1		340.06	
Glutamine		5	10	3	2			146.06	1		339.08	
Glycine		2	5	2	1			75.03			226.00	
Histidine		6	9	2	3			155.06		1	502.01	
Isoleucine		6	13	2	1			131.08			282.06	
Leucine		6	13	2	1			131.08			282.06	
Lysine		6	14	2	2			146.09		1	493.04	
Me.Histidine		7	11	2	3			169.08			320.05	
Methionine		5	11	2	1	1		149.04			300.02	
OH-Lysine		6	14	3	2			162.09		2	705.01	
OH-Proline		5	9	3	1			131.05		1	478.00	
Ornithine		5	12	2	2			132.08		1	479.03	
Phenylalanine		9	11	2	1			165.07			316.05	
Proline		5	9	2	1			115.06			266.03	
Pyroglutamate		5	7	3	1			129.04		-1	84.04	
Serine		3	7	3	1			105.04		1	451.99	
Threonine		4	9	3	1			119.05		1	466.00	
Tryptophan		11	12	2	2			204.08			355.06	
Tyrosine		9	11	3	1			181.06		1	528.02	
Valine		5	11	2	1			117.07			268.05	
DABA = 2,4-diaminobutyrate												

Heptafluorobutyryl <i>n</i> -Propyl (HFBP) Derivative / CI Ionization													
											M=AA+HFB+Pr		
											HFB+Pr=	238.02	
		Composition						MW	Add deriv units:		NCI		PCI
	atom:	C	H	O	N	S		(AA)	Propyl-	HFB-	[M-HF] ⁺	[M-COOPrH] ⁺	[M+H] ⁺
Species	mass:	12	1	16	14	32			on COOH	on NH2, OH, SH			
	defect:	0	0.007	-0.005	0.003	-0.028			42.04	195.97	-20.01	-88.05	1.007
Alanine		3	7	2	1			89.04			307.05	239.01	328.06
Arginine		6	14	2	4			174.10		2	784.06	716.02	805.07
Asparagine		4	8	3	2			132.05	1		392.10	324.06	413.11
Aspartate		4	7	4	1			133.03	1		393.08	325.04	414.10
Cysteine		3	7	2	1	1		121.01		1	535.00	466.96	556.01
DABA													
Glutamate		5	9	4	1			147.05	1		407.10	339.06	428.11
Glutamine		5	10	3	2			146.06	1		406.11	338.07	427.13
Glycine		2	5	2	1			75.03			293.04	225.00	314.05
Histidine		6	9	2	3			155.06		1	569.05	501.01	590.06
Isoleucine		6	13	2	1			131.08			349.09	281.05	370.11
Leucine		6	13	2	1			131.08			349.09	281.05	370.11
Lysine		6	14	2	2			146.09		1	560.08	492.04	581.09
Me.Histidine		7	11	2	3			169.08			387.09	319.05	408.10
Methionine		5	11	2	1	1		149.04			367.05	299.01	388.06
OH-Lysine		6	14	3	2			162.09		2	772.05	704.01	793.06
OH-Proline		5	9	3	1			131.05		1	545.04	476.99	566.05
Ornithine		5	12	2	2			132.08		1	546.06	478.02	567.08
Phenylalanine		9	11	2	1			165.07			383.08	315.04	404.09
Proline		5	9	2	1			115.06			333.07	265.03	354.08
Pyroglutamate		5	7	3	1			129.04		-1	151.07	83.03	172.09
Serine		3	7	3	1			105.04		1	519.02	450.98	540.03
Threonine		4	9	3	1			119.05		1	533.04	464.99	554.05
Tryptophan		11	12	2	2			204.08			422.09	354.05	443.10
Tyrosine		9	11	3	1			181.06		1	595.05	527.01	616.06
Valine		5	11	2	1			117.07			335.08	267.04	356.09
Urea		1	4	1	2			60.03	-1	1	431.97		452.98
DABA = 2,4-diaminobutyrate													

N-Acetyl <i>n</i> -Propyl (NAP) Derivative / EI Ionization												
											M=AA+Ac+Pr	
											Ac+Pr=	84.05
		Composition						MW (AA)	Add deriv units:			
Species	atom: mass: defect:	C	H	O	N	S			Propyl- on COOH	Acetyl- on NH ₂ , OH, SH	[M] ⁺	[M-COOPr] ⁺
		12	1	16	14	32						
		0	0.007	-0.005	0.003	-0.028			42.04	42.01		-87.04
Alanine		3	7	2	1			89.04			173.09	86.05
Arginine		6	14	2	4			174.10		2	342.17	255.13
Asparagine		4	8	3	2			132.05	1		258.14	171.10
Aspartate		4	7	4	1			133.03	1		259.12	172.09
Cysteine		3	7	2	1	1		121.01		1	247.07	160.03
DABA												
Glutamate		5	9	4	1			147.05	1		273.14	186.10
Glutamine		5	10	3	2			146.06	1		272.15	185.11
Glycine		2	5	2	1			75.03			159.08	72.04
Histidine		6	9	2	3			155.06		1	281.12	194.08
Isoleucine		6	13	2	1			131.08			215.13	128.10
Leucine		6	13	2	1			131.08			215.13	128.10
Lysine		6	14	2	2			146.09		1	272.15	185.11
Me.Histidine		7	11	2	3			169.08			253.13	166.09
Methionine		5	11	2	1	1		149.04			233.09	146.05
OH-Lysine		6	14	3	2			162.09		2	330.16	243.12
OH-Proline		5	9	3	1			131.05		1	257.11	170.07
Ornithine		5	12	2	2			132.08		1	258.14	171.10
Phenylalanine		9	11	2	1			165.07			249.12	162.08
Proline		5	9	2	1			115.06			199.11	112.07
Pyroglutamate		5	7	3	1			129.04		-1	171.08	84.04
Serine		3	7	3	1			105.04		1	231.10	144.06
Threonine		4	9	3	1			119.05		1	245.11	158.07
Tryptophan		11	12	2	2			204.08			288.13	201.09
Tyrosine		9	11	3	1			181.06		1	307.12	220.09
Valine		5	11	2	1			117.07			201.12	114.08
Urea		1	4	1	2			60.03	-1	1	144.05	
DABA = 2,4-diaminobutyrate												