

t-Butyldimethylsilyl (tBDMS)-Derivative / EI Ionization														
													M=AA+2*tBDMS	
													2*tBDMS= 228.15	
Composition							MW	Add deriv units:						
Species	atom:	C	H	O	N	S	(AA)	tBDMS-	tBDMS-	[M]⁺	[M-tB]⁺	[M-COOtBDMS]⁺	[M-COtB]⁺	
	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		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		463.24	406.17	304.17	378.18	
DABA		4	10	2	2			118.07		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		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		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		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		618.38	561.32	459.31	533.33	
OH-Proline		5	9	3	1			131.05		473.27	416.21	314.20	388.21	
Ornithine		5	12	2	2			132.08		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		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		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		516.31	459.25	357.24	431.25	
Threonine		4	9	3	1			119.05		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		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	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														