

**Relative and Fractional Abundance of Derivatives**

calculated by: Mass Spec Ion Abundance Calculator (Ver 4.1)

Ionization: EI

Ion: [M - t-butyl]<sup>+</sup>

Derivative: tBDMS

Species	Number of Atoms							mass	mass defect	Relative Abundance [%]							Fractional Abundance [%]						
	C	H	O	N	S	F	Si			M	M+1	M+2	M+3	M+4	M+5	M+6	M	M+1	M+2	M+3	M+4	M+5	M+6
Alanine	11	26	2	1	0	0	2	260	0.127	100	23.07	9.45	1.44	0.25	0.03	74.50	17.19	7.04	1.07	0.19	0.02		
Arginine	26	61	2	4	0	0	4	573	0.333	100	51.32	26.30	8.33	2.35	0.52	0.10	52.93	27.16	13.92	4.41	1.24	0.27	0.05
Asparagine	18	41	3	2	0	0	3	417	0.206	100	36.46	16.82	4.02	0.94	0.16	0.02	63.12	23.02	10.62	2.54	0.59	0.10	0.01
Aspartate	18	40	4	1	0	0	3	418	0.191	100	36.12	16.90	4.03	0.96	0.16	0.02	63.21	22.83	10.68	2.55	0.61	0.10	0.02
Cysteine	17	40	2	1	1	0	3	406	0.173	100	35.74	20.79	5.37	1.61	0.31	0.06	61.02	21.80	12.68	3.28	0.98	0.19	0.04
Glutamate	19	42	4	1	0	0	3	432	0.205	100	37.24	17.30	4.22	1.01	0.17	0.03	62.51	23.28	10.82	2.64	0.63	0.11	0.02
Glutamine	19	43	3	2	0	0	3	431	0.220	100	37.59	17.23	4.21	0.99	0.17	0.02	62.42	23.46	10.75	2.63	0.62	0.10	0.02
Glycine	10	24	2	1	0	0	2	246	0.113	100	21.95	9.20	1.33	0.24	0.02	75.34	16.53	6.93	1.01	0.18	0.02		
Histidine	20	42	2	3	0	0	3	440	0.221	100	39.00	17.56	4.37	1.01	0.17	0.03	61.68	24.05	10.83	2.70	0.62	0.11	0.02
Isoleucine	14	32	2	1	0	0	2	302	0.169	100	26.45	10.26	1.77	0.30	0.03	72.04	19.05	7.39	1.27	0.22	0.02		
Leucine	14	32	2	1	0	0	2	302	0.169	100	26.45	10.26	1.77	0.30	0.03	72.04	19.05	7.39	1.27	0.22	0.02		
Lysine	20	47	2	2	0	0	3	431	0.253	100	38.70	17.44	4.32	1.00	0.17	0.02	61.86	23.94	10.79	2.67	0.62	0.10	0.02
Me.Histidine	15	30	2	3	0	0	2	340	0.161	100	28.25	10.75	1.95	0.34	0.04	70.76	19.99	7.61	1.38	0.24	0.03		
Methionine	13	30	2	1	1	0	2	320	0.127	100	26.11	14.62	2.86	0.76	0.11	0.02	69.22	18.07	10.12	1.98	0.52	0.08	0.01
OH-Lysine	26	61	3	2	0	0	4	561	0.322	100	50.62	26.15	8.25	2.35	0.52	0.10	53.19	26.92	13.91	4.39	1.25	0.28	0.05
OH-Proline	19	42	3	1	0	0	3	416	0.210	100	37.20	17.08	4.14	0.97	0.16	0.02	62.66	23.31	10.71	2.60	0.61	0.10	0.02
Ornithine	19	45	2	2	0	0	3	417	0.239	100	37.58	17.02	4.13	0.95	0.16	0.02	62.56	23.51	10.65	2.58	0.60	0.10	0.01
Phenylalanine	17	30	2	1	0	0	2	336	0.155	100	29.70	11.16	2.11	0.36	0.04	69.74	20.72	7.78	1.47	0.25	0.03		
Proline	13	28	2	1	0	0	2	286	0.141	100	25.29	9.97	1.65	0.28	0.03	72.87	18.43	7.27	1.20	0.21	0.02		
Pyroglutamate	7	12	3	1	0	0	1	186	0.048	100	13.43	4.69	0.38	0.04		84.36	11.33	3.96	0.32	0.03			
Serine	17	40	3	1	0	0	3	390	0.196	100	34.98	16.30	3.78	0.89	0.14	0.02	64.06	22.41	10.44	2.42	0.57	0.09	0.01
Threonine	18	42	3	1	0	0	3	404	0.210	100	36.11	16.69	3.96	0.93	0.15	0.02	63.35	22.87	10.57	2.51	0.59	0.10	0.01
Tryptophan	19	31	2	2	0	0	2	375	0.165	100	32.28	11.95	2.40	0.42	0.05	67.98	21.94	8.12	1.63	0.29	0.04		
Tyrosine	23	44	3	1	0	0	3	466	0.224	100	41.62	18.80	4.92	1.17	0.21	0.03	59.97	24.96	11.27	2.95	0.70	0.13	0.02
Valine	13	30	2	1	0	0	2	288	0.155	100	25.32	9.98	1.65	0.28	0.03	72.85	18.45	7.27	1.20	0.21	0.02		
Urea	9	23	1	2	0	0	2	231	0.114	100	21.17	8.83	1.22	0.21	0.02	76.08	16.10	6.72	0.93	0.16	0.01		
KIC	14	19	1	2	0	0	1	259	0.110	100	21.49	5.65	0.72	0.06		78.18	16.80	4.42	0.56	0.05			
KIV	13	17	1	2	0	0	1	245	0.096	100	20.37	5.42	0.66	0.05		79.05	16.10	4.29	0.52	0.04			
KC	14	19	1	2	0	0	1	259	0.110	100	21.49	5.65	0.72	0.06		78.18	16.80	4.42	0.56	0.05			

**Relative and Fractional Abundance of Derivatives**

calculated by: Mass Spec Ion Abundance Calculator (Ver 4.1)

Ionization: EI

Derivative: tBDMS

Ion: [M - COOtBDMS]<sup>+</sup>

Species	Number of Atoms							mass	mass defect	Relative Abundance [%]							Fractional Abundance [%]						
	C	H	O	N	S	F	Si			M	M+1	M+2	M+3	M+4	M+5	M+6	M	M+1	M+2	M+3	M+4	M+5	M+6
Alanine	8	20	1	1	0	0	0	158	0.119	100	14.52	4.23	0.35	0.01			83.96	12.19	3.55	0.29	0.01		
Arginine	23	55	4	3	0	0	0	471	0.325	100	42.77	18.67	4.88	1.11	0.19	0.03	59.65	25.51	11.14	2.91	0.66	0.11	0.02
Asparagine	15	35	1	2	0	0	2	315	0.198	100	27.92	10.45	1.86	0.31	0.03		71.14	19.86	7.44	1.32	0.22	0.02	
Aspartate	15	34	2	1	0	0	2	316	0.183	100	27.57	10.56	1.88	0.32	0.04		71.24	19.64	7.52	1.34	0.23	0.03	
Cysteine	14	34	1	1	0	0	2	304	0.165	100	27.19	14.49	2.90	0.73	0.11	0.02	68.76	18.70	9.96	2.00	0.50	0.07	0.01
Glutamate	16	36	2	1	0	0	2	330	0.197	100	28.70	10.87	2.00	0.34	0.04		70.45	20.21	7.66	1.41	0.24	0.03	
Glutamine	16	37	1	2	0	0	2	329	0.212	100	29.04	10.77	1.98	0.33	0.04		70.35	20.43	7.57	1.39	0.23	0.03	
Glycine	7	18	1	1	0	0	0	144	0.105	100	13.40	4.08	0.30			84.90	11.38	3.46	0.26				
Histidine	17	36	3	2	0	0	0	338	0.213	100	30.45	10.98	2.07	0.33	0.04		69.51	21.17	7.63	1.44	0.23	0.03	
Isoleucine	11	26	1	1	0	0	0	200	0.161	100	17.90	4.76	0.49	0.03			81.19	14.53	3.86	0.40	0.02		
Leucine	11	26	1	1	0	0	0	200	0.161	100	17.90	4.76	0.49	0.03			81.19	14.53	3.86	0.40	0.02		
Lysine	17	41	2	2	0	0	0	329	0.245	100	30.16	10.89	2.04	0.33	0.04		69.71	21.02	7.59	1.42	0.23	0.03	
Me.Histidine	12	24	3	1	0	0	0	238	0.153	100	19.70	5.09	0.58	0.04			79.74	15.71	4.06	0.46	0.03		
Methionine	10	24	1	1	0	0	1	218	0.119	100	17.56	9.14	1.22	0.25	0.02		78.01	13.70	7.13	0.95	0.19	0.02	
OH-Lysine	23	55	1	2	0	0	3	459	0.314	100	42.07	18.58	4.84	1.11	0.19	0.03	59.95	25.22	11.14	2.90	0.67	0.12	0.02
OH-Proline	16	36	1	1	0	0	2	314	0.202	100	28.66	10.66	1.94	0.32	0.04		70.62	20.24	7.53	1.37	0.23	0.03	
Ornithine	16	39	2	2	0	0	0	315	0.231	100	29.03	10.56	1.92	0.31	0.03		70.50	20.47	7.44	1.35	0.22	0.02	
Phenylalanine	14	24	1	1	0	0	0	234	0.147	100	21.16	5.37	0.66	0.05			78.60	16.63	4.22	0.52	0.04		
Proline	10	22	1	1	0	0	0	184	0.133	100	16.74	4.56	0.44	0.02			82.12	13.75	3.75	0.36	0.02		
Pyroglutamate	4	6	1	1	0	0	0	84	0.040	100	4.88	0.30	0.01				95.07	4.64	0.28	0.01			
Serine	14	34	1	1	0	0	2	288	0.188	100	26.44	10.06	1.71	0.28	0.03		72.19	19.09	7.26	1.24	0.20	0.02	
Threonine	15	36	1	1	0	0	2	302	0.202	100	27.56	10.35	1.82	0.30	0.03		71.39	19.68	7.39	1.30	0.22	0.02	
Tryptophan	16	25	2	1	0	0	0	273	0.157	100	23.73	5.94	0.80	0.06			76.61	18.18	4.55	0.61	0.05		
Tyrosine	20	38	1	1	0	0	2	364	0.216	100	33.07	11.99	2.43	0.41	0.05		67.58	22.35	8.11	1.64	0.28	0.04	
Valine	10	24	1	1	0	0	0	186	0.147	100	16.77	4.57	0.44	0.02			82.10	13.77	3.75	0.36	0.02		