Appendix A

Below is a summary table of the side-chain assignments of the apo N-terminal domain.

Hsp90 N-terminal domain - Apo state		Chemical Shift	
Carbon Assignment	Proton Assignment	C(ppm)	H(ppm)
1MetCa	1MetHa	55.038	4.556
1MetCg	1MetHg*	31.650	2.596
1Met[1916]	1MetHbb	32.466	2.116
3SerCa	3SerHa	57.733	4.959
3SerCb	3SerHbb	64.433	3.726
3SerCb	3SerHba	64.432	3.711
4GluCa	4GluHa	55.385	4.510
4GluCb	4Glu[1931]	33.410	2.317
4GluCb	4GluHbb	33.941	1.939
4GluCb	4GluHba	33.941	1.900
4GluCg	4GluHga	36.464	2.306
4GluCg	4GluHgb	36.456	2.331
5ThrCa	5ThrHa	61.475	4.791
5ThrCb	5ThrHb	69.950	3.650
5ThrCg2	5ThrHg2*	20.651	1.000
7GluCa	7GluHa	55.074	4.686
7GluCb	7GluHbb	30.583	2.391
7GluCb	7GluHba	30.600	2.114
7GluCg	7GluHgb	36.941	2.285
7GluCg	7GluHga	36.885	2.162
8PheCa	8PheHa	59.438	4.779
8PheCb	8PheHba	40.291	2.940
11GluCa	11GluHa	60.296	4.042
11GluCg	11GluHgb	37.528	2.468
11GluCg	11GluHga	37.522	2.367
12IleCa	12IleHa	63.831	3.512
12IleCb	12IleHb	36.948	2.075
12IleCd1	12IleHd1*	12.607	0.970
12IleCg2	12IleHg2*	17.947	0.556
13ThrCa	13ThrHa	66.400	3.864
13ThrCb	13ThrHb	67.817	4.206
13ThrCg2	13ThrHg2*	23.096	1.170

14GlnCa	14GlnHa	58.634	3.991
14GlnCa	14GlnH	58.553	7.936
14GlnCb	14GlnHba	27.287	1.979
14GlnCb	14GlnHbb	27.295	2.121
14GlnCg	14GlnHga	33.182	2.378
14GlnCg	14GlnHgb	33.180	2.499
15LeuCa	15LeuHa	58.129	4.042
15LeuCda	15LeuHda*	25.917	0.865
15LeuCg	15LeuHg	25.068	1.522
15Leu[2653]	15Leu[3781]	58.042	4.108
17SerCa	17SerHa	61.302	4.116
17SerCb	17SerHbb	62.563	3.962
17SerCb	17SerHba	62.541	3.922
18Leu([1810]/Cg)	18Leu([1813]/Hg)	26.492	1.658
18LeuCa	18LeuHa	57.787	4.158
18LeuCb	18LeuHba	41.825	1.857
18LeuCda	18LeuHda*	24.187	0.813
18LeuCg	18LeuHg	26.754	1.670
19IleCa	19IleHa	64.135	3.683
19IleCb	19IleHb	36.569	2.039
19IleCd1	19IleHd1*	11.925	0.757
19IleCg1	19IleHg1a	28.234	1.665
19IleCg2	19IleHg2*	17.599	0.965
20IleCa	20IleHa	64.405	3.987
20IleCb	20IleHb	37.495	1.891
20IleCd1	20IleHd1*	13.572	0.906
20IleCg1	20IleHg1a	29.070	1.442
20IleCg2	20IleHg2*	16.478	1.010
21AsnCa	21AsnHa	53.624	4.929
21AsnCb	21AsnHbb	40.267	2.921
21AsnCb	21AsnHba	40.267	2.776
22ThrCa	22ThrHa	59.579	4.337
26AsnCb	26AsnHba	37.544	3.004
26AsnCb	26AsnHbb	37.547	3.063
27LysCa	27LysHa	59.639	3.982
27LysCb	27LysHbb	31.768	1.972
27LysCb	27LysHba	31.770	1.843
27LysCd	27LysHda	28.839	1.709
27LysCe	27LysHea	41.547	3.039
27LysCg	27LysHga	24.324	1.447
27LysCg	27LysHgb	24.324	1.554
28GluCa	28GluHa	58.376	4.131
28GluCg	28GluHga	34.386	1.931
29IleCa	29IleHa	62.338	3.568
29IleCb	29IleHb	37.896	2.133

29IleCd1	29IleHd1*	14.414	0.787
29IleCg1	29IleHg1b	25.968	1.533
29IleCg1	29IleHg1a	25.953	1.435
29IleCg2	29IleHg2*	19.651	0.987
30PheCa	30PheHa	59.239	4.453
30PheCb	30PheHba	37.165	2.672
31LeuCa	31LeuHa	56.633	3.110
31LeuCb	31LeuHbb	40.527	1.197
31LeuCb	31LeuHba	40.536	0.340
31LeuCda	31LeuHda*	24.896	0.706
31LeuCdb	31LeuHdb*	23.423	0.729
32ArgCa	32ArgHa	58.471	3.655
32ArgCb	32ArgHba	28.189	1.811
32ArgCd	32ArgHdb	43.244	3.075
32ArgCd	32ArgHda	43.265	3.044
32ArgCg	32ArgHga	25.157	1.455
33GluCa	33GluHa	57.710	4.037
33GluCb	33GluHbb	27.870	2.153
33GluCb	33GluHba	27.820	2.107
33GluCg	33GluHgb	35.392	2.202
33GluCg	33GluHga	35.387	2.155
34LeuCb	34LeuHba	39.099	1.860
34LeuCda	34LeuHda*	26.375	0.949
35?IleCD1[4049]	35?Ile[4050]	12.710	0.755
35IleCa	35IleHa	65.178	3.693
35IleCb	35IleHb	35.425	2.025
35IleCd1	35IleHd1*	13.884	0.813
35IleCg2	35IleHg2*	16.811	0.981
36SerCa	36SerHa	61.808	4.276
36SerCb	36SerHba	62.326	4.021
37AsnCa	37AsnHa	55.631	4.391
37AsnCb	37AsnHba	37.643	2.901
38AlaCa	38AlaHa	54.589	4.142
38AlaCb	38AlaHb*	18.030	1.525
38AlaCb	38AlaHb*	17.722	1.513
39SerCa	39SerHa	61.532	4.054
39SerCb	39SerHba	62.508	4.065
40AspCa	40AspHa	57.338	4.430
40AspCb	40AspHba	40.305	2.740
40AspCb	40AspHbb	40.305	2.922
41AlaCa	41AlaHa	55.000	4.159
41AlaCb	41AlaHb*	18.069	1.662
42LeuCa	42LeuHa	57.391	3.880
42LeuCb	42LeuHbb	39.880	1.642
42LeuCb	42LeuHba	39.920	1.617

42LeuCda	42LeuHdb*	24.732	0.387
42LeuCdb	42LeuHda*	25.012	0.116
42LeuCg	42LeuHg	26.486	1.213
43AspCa	43AspHa	57.589	4.274
43AspCb	43AspHba	39.310	2.711
44LysCa	44LysHa	60.120	4.175
44LysCb	44LysHba	32.499	1.914
44LysCb	44LysHbb	32.512	2.100
44LysCd	44LysHda	29.017	1.694
44LysCe	44LysHea	41.752	2.972
44LysCg	44LysHga	26.078	1.689
45IleCa	45IleHa	59.690	4.554
45IleCb	45IleHb	38.147	1.461
45IleCd1	45IleHd1*	13.963	1.020
45IleCg1	45IleHg1a	28.933	1.265
45IleCg2	45IleHg2*	20.070	1.322
46ArgCa	46ArgHa	60.020	3.928
46ArgCb	46ArgHbb	29.399	1.919
46ArgCb	46ArgHba	29.381	1.816
46ArgCd	46ArgHda	43.480	3.291
46ArgCd	46ArgHdb	43.478	3.450
46ArgCg	46ArgHgb	26.466	1.572
46ArgCg	46ArgHga	26.485	1.438
47TyrCa	47TyrHa	60.948	4.349
47TyrCb	47TyrHbb	37.281	3.217
47TyrCb	47TyrHba	37.278	3.149
48LysCa	48LysHa	59.028	4.069
48LysCb	48LysHba	32.448	1.922
48LysCb	48LysHbb	32.448	2.117
48LysCd	48LysHdb	29.087	1.540
48LysCd	48LysHda	29.072	1.438
48LysCe	48LysHea	41.423	3.037
48LysCg	48LysHgb	25.050	1.717
48LysCg	48LysHga	25.047	1.532
49SerCa	49SerHa	59.980	4.380
50LeuCa	50LeuHa	57.128	4.173
50LeuCb	50LeuHbb	40.929	1.872
50LeuCb	50LeuHba	40.901	1.524
50LeuCda	50LeuHda*	21.751	0.903
50LeuCdb	50LeuHdb*	24.803	0.989
50LeuCg	50LeuHg	25.723	2.057
51SerCa	51SerHa	58.145	4.646
51SerCb	51SerHbb	63.656	3.989
51SerCb	51SerHba	63.629	3.899
52AspCa	52AspHa	51.372	5.118

52AspCb	52AspHba	40.946	2.638
52AspCb	52AspHbb	40.945	2.861
54LysCb	54LysHba	30.838	1.903
54LysCb	54LysHbb	30.836	2.033
54LysCd	54LysHda	28.218	1.738
54LysCe	54LysHea	41.314	3.053
54LysCg	54LysHga	24.288	1.472
54LysCg	54LysHgb	24.286	1.544
55GlnCa	55GlnHa	56.879	3.809
55GlnCb	55GlnHbb	26.557	1.994
55GlnCb	55GlnHba	26.561	1.918
55GlnCg	55GlnHga	32.984	2.230
55GlnCg	55GlnHgb	32.954	2.679
56LeuCa	56LeuHa	54.735	4.272
56LeuCb	56LeuHba	42.413	1.809
56LeuCb	56LeuHba	42.412	1.777
56LeuCda	56LeuHda*	23.233	0.900
56LeuCda	56LeuHdb*	24.336	1.050
57GluCa	57GluHa	59.096	3.895
57GluCb	57GluHba	28.860	1.724
57GluCg	57GluHga	36.638	2.407
58ThrCa	58ThrHa	62.077	3.972
58ThrCb	58ThrHb	68.793	4.356
58ThrCg2	58ThrHg2*	22.514	1.313
59GluCb	59GluHba	29.140	2.091
59GluCb	59GluHbb	29.125	2.290
59GluCg	59GluHgb	37.521	2.513
59GluCg	59GluHga	37.481	2.263
62?LeuCD2|CD1[1570]	62?Leu[1571]	20.144	0.657
62?Leu[1669]	62?LeuHD2*|HD1*[1670]	20.253	1.038
62LeuCa	62LeuHa	53.411	4.275
62LeuCb	62LeuHbb	40.123	2.129
62LeuCb	62LeuHba	40.252	1.226
62LeuCda	62LeuHda*	23.355	0.678
62LeuCg	62LeuHg	25.563	1.795
63PheCa	63PheHa	56.079	5.033
63PheCb	63PheHba	41.429	3.002
64IleCa	64IleHa	60.006	4.995
64IleCb	64IleHb	39.962	1.805
64IleCd1	64IleHd1*	13.896	0.830
64IleCg2	64IleHg2*	16.076	0.830
65ArgCa	65ArgHa	54.341	5.627
65ArgCb	65ArgHba	33.049	1.704
65ArgCd	65ArgHdb	42.851	3.257
65ArgCd	65ArgHda	42.855	3.210

65ArgCg	65ArgHga	26.548	1.719
66IleCa	66IleHa	60.178	5.098
66IleCb	66IleHb	39.092	1.893
66IleCd1	66IleHd1*	13.892	0.819
66IleCg1	66IleHg1a	27.148	1.569
66IleCg2	66IleHg2*	17.625	0.975
67ThrCa	67ThrHa	59.195	4.914
67ThrCb	67ThrHb	71.453	4.044
67ThrCg2	67ThrHg2*	20.731	1.213
69LysCb	69LysHba	31.531	1.919
69LysCd	69LysHda	28.978	1.591
69LysCe	69LysHea	41.543	3.017
69LysCg	69LysHga	24.065	1.286
71GluCa	71GluHa	58.898	4.229
71GluCb	71GluHba	27.574	2.016
71GluCb	71GluHbb	27.574	2.143
71GluCg	71GluHga	36.148	2.357
71GluCg	71GluHgb	36.155	2.478
72GlnCa	72GlnHa	55.033	4.515
72GlnCb	72GlnHbb	29.547	2.285
72GlnCb	72GlnHba	29.547	2.238
72GlnCg	72GlnHga	35.687	2.281
72GlnCg	72GlnHgb	35.671	2.448
73LysCb	73LysHba	28.781	1.811
73LysCe	73LysHea	41.545	3.105
73LysCg	73LysHga	25.115	1.480
74ValCa	74ValHa	58.582	5.140
74ValCb	74ValHb	36.617	1.490
74ValCga	74ValHga*	22.021	0.308
74ValCgb	74ValHgb*	22.554	0.535
75LeuCa	75LeuHa	53.002	4.757
75LeuCda	75LeuHda*	22.442	0.985
75LeuCg	75LeuHg	25.214	1.092
76GluCa	76GluHa	54.108	5.788
76GluCb	76GluHba	30.745	2.114
76GluCg	76GluHgb	37.479	2.241
76GluCg	76GluHga	37.478	1.920
77IleCa	77IleHa	60.867	4.739
77IleCb	77IleHb	40.016	1.862
77IleCd1	77IleHd1*	15.302	0.871
77IleCg1	77IleHg1b	27.245	1.613
77IleCg1	77IleHg1a	27.242	1.540
77Ile[1554]	77IleHg2*	17.371	0.758
79AspCa	79AspHa	52.313	5.634
80SerCa	80SerHa	54.351	5.233

80SerCb	80SerHba	62.101	4.111
81GlyCa	81GlyHab	44.092	4.093
81GlyCa	81GlyHaa	44.096	4.069
82IleCa	82IleHa	62.688	3.782
82IleCb	82IleHb	39.408	1.639
82IleCd1	82IleHd1*	13.535	0.829
82IleCg1	82IleHg1a	29.070	1.456
82IleCg2	82IleHg2*	15.635	1.210
84MetCa	84MetHa	54.233	4.955
84MetCb	84MetHba	36.476	1.687
84MetCg	84MetHga	33.332	2.134
85ThrCa	85ThrHa	60.193	4.713
85ThrCb	85ThrHb	70.194	5.010
85ThrCg2	85ThrHg2*	21.876	1.343
87AlaCa	87AlaHa	54.500	3.912
87AlaCb	87AlaHb*	17.503	1.310
88GluCa	88GluHa	58.893	3.844
88GluCb	88GluHba	29.215	2.123
88GluCb	88GluHbb	29.207	2.371
88GluCg	88GluHgb	37.530	2.494
90IleCa	90IleHa	65.242	3.424
90IleCa	90IleHa	65.235	3.403
90IleCb	90IleHb	38.835	1.567
90IleCd1	90IleHd1*	15.266	0.609
90IleCg1	90IleHg1a	29.352	1.427
90IleCg2	90IleHg2*	16.528	0.528
91AsnCa	91AsnHa	55.481	4.585
91AsnCb	91AsnHbb	38.869	2.780
91AsnCb	91AsnHba	38.867	2.657
92AsnCa	92AsnHa	57.623	4.610
92AsnCb	92AsnHba	39.938	2.803
92AsnCb	92AsnHbb	39.940	2.921
93?LeuCB[4419]	93?LeuHB2|HB3[4421]	38.956	1.168
93?LeuCB[4419]	93?LeuHB2|HB3[4420]	38.988	0.524
93LeuCa	93LeuHa	54.196	4.224
93LeuCda	93LeuHda*	19.252	-0.704
93LeuCdb	93LeuHdb*	23.063	-0.776
93LeuCg	93LeuHg	24.862	0.698
94GlyCa	94GlyHab	47.261	4.352
94GlyCa	94GlyHaa	47.261	3.461
95ThrCa	95ThrHa	63.599	4.831
95ThrCb	95ThrHb	70.700	4.513
95ThrCg2	95ThrHg2*	21.341	1.401
96?IleCA[1499]	96?IleHD1*[1500]	12.232	0.879
96IleCa	96IleHa	61.510	4.481

96IleCb	96IleHb	41.761	1.801
96IleCd1	96IleHd1*	15.132	0.906
96IleCg2	96IleHg2*	17.580	0.983
101ThrCa	101ThrHa	63.463	4.367
101ThrCb	101ThrHb	69.146	4.346
101ThrCg2	101ThrHg2*	20.478	1.235
103AlaCa	103AlaHa	54.541	4.194
103AlaCb	103AlaHb*	17.645	1.711
103Ala[1608]	103AlaHb*	17.396	1.758
104PheCa	104PheHa	58.586	5.086
105MetCa	105MetHa	59.477	4.003
105MetCb	105MetHbb	31.803	1.975
105MetCb	105MetHba	31.790	1.837
105MetCg	105MetHga	28.629	2.001
106GluCa	106GluHa	59.005	3.948
106GluCb	106GluHba	28.652	2.118
106GluCg	106GluHga	36.140	2.243
106GluCg	106GluHgb	36.165	2.465
107AlaCa	107AlaHa	54.735	4.163
107AlaCb	107AlaHb*	16.540	1.389
108LeuCa	108LeuHa	57.419	4.141
108LeuCb	108LeuHbb	40.918	1.885
108LeuCb	108LeuHba	40.918	1.534
108LeuCda	108LeuHda*	21.289	0.907
108LeuCdb	108LeuHdb*	24.193	1.002
109SerCa	109SerHa	60.955	4.261
109SerCb	109SerHba	62.602	4.000
110AlaCa	110AlaHa	51.362	4.574
110AlaCb	110AlaHb*	18.323	1.527
111GlyCa	111GlyHaa	44.981	3.786
111GlyCa	111GlyHab	44.971	4.461
112AlaCa	112AlaHa	51.925	4.402
112AlaCb	112AlaHb*	18.729	1.297
113AspCa	113AspHa	53.027	4.840
113AspCb	113AspHbb	43.883	2.910
113AspCb	113AspHba	43.885	2.748
114?/23?ValCG2|CG1[1719]	114?/23?ValHG2*|HG1*[1720]	26.666	-0.012
114?/23?ValCG2|CG1[1721]	114?/23?ValHG2*|HG1*[1722]	23.090	-0.514
115SerCa	115SerHa	60.711	4.093
115SerCb	115SerHba	62.962	4.389
116MetCa	116MetHa	56.126	4.547
116MetCb	116MetHba	31.968	2.542
116MetCg	116MetHgb	30.677	3.216

116MetCg	116MetHga	30.671	3.194
117IleCa	117IleHa	65.065	2.998
117IleCb	117IleHb	37.010	1.935
117IleCd1	117IleHd1*	14.772	0.818
117IleCg2	117IleHg2*	19.627	0.980
118GlyCa	118GlyHaa	46.308	3.839
118GlyCa	118GlyHab	46.298	4.220
119GlnCa	119GlnHa	56.983	4.124
119GlnCb	119GlnHba	27.262	1.909
119GlnCg	119GlnHga	33.415	2.245
119GlnCg	119GlnHgb	33.407	2.313
120PheCb	120PheHbb	39.353	3.243
120PheCb	120PheHba	39.353	2.758
121GlyCa	121GlyHaa	46.243	4.073
121GlyCa	121GlyHab	46.254	4.186
122ValCa	122ValHa	59.386	5.015
122ValCb	122ValHb	30.603	2.819
122ValCga	122ValHga*	17.282	0.606
123GlyCa	123GlyHaa	47.278	3.488
123GlyCa	123GlyHab	47.254	4.306
124PheCa	124PheHa	60.853	4.752
124PheCb	124PheHba	40.004	2.956
125TyrCa	125TyrHa	60.889	3.909
125TyrCb	125TyrHbb	37.167	2.869
125TyrCb	125TyrHba	37.161	2.817
126SerCa	126SerHa	61.675	3.897
126SerCb	126SerHba	62.926	3.984
127LeuCa	127LeuHa	57.838	3.827
127LeuCb	127LeuHba	40.137	1.736
127LeuCda	127LeuHda*	23.000	0.729
127LeuCdb	127LeuHdb*	23.024	1.084
127LeuCg	127LeuHg	26.533	1.360
128PheCa	128PheHa	60.519	5.027
128PheCb	128PheHba	37.112	2.843
128PheCb	128PheHbb	37.112	3.519
129LeuCa	129LeuHa	57.149	4.298
129LeuCb	129LeuHba	42.468	1.752
129LeuCda	129LeuHda*	24.810	0.857
130ValCa	130ValHa	60.104	4.601
130ValCb	130ValHb	32.690	2.060
130ValCgb	130ValHga*	14.661	-0.568
130ValCgb	130ValHgb*	21.507	0.490
131AlaCa	131AlaHa	50.622	5.081
131AlaCb	131AlaHb*	21.653	1.090
133ArgCa	133ArgHa	54.670	5.134

133ArgCb	133ArgHba	32.660	1.807
133ArgCd	133ArgHdb	42.910	2.797
133ArgCd	133ArgHda	42.913	2.566
133ArgCg	133ArgHga	26.449	1.555
133ArgCg	133ArgHgb	26.453	1.688
134ValCa	134ValHa	58.335	5.793
134ValCb	134ValHb	34.782	1.956
134ValCga	134ValHga*	21.711	1.001
134ValCgb	134ValHgb*	20.066	1.327
136ValCa	136ValHa	61.325	4.938
136ValCb	136ValHb	32.370	2.422
136ValCga	136ValHga*	20.954	0.716
137IleCa	137IleHa	59.840	5.258
137IleCb	137IleHb	39.110	1.923
137IleCd1	137IleHd1*	14.380	0.874
137IleCg1	137IleHg1b	29.057	1.592
137IleCg1	137IleHg1a	28.994	1.174
137IleCg2	137IleHg2*	18.855	1.028
138SerCa	138SerHa	56.924	5.616
138SerCb	138SerHbb	66.815	3.932
138SerCb	138SerHba	66.781	3.508
140SerCa	140SerHa	54.731	5.009
140SerCb	140SerHba	63.368	3.382
140SerCb	140SerHbb	63.358	3.618
141AsnCa	141AsnHa	54.988	4.451
141AsnCb	141AsnHba	36.599	2.865
142AspCa	142AspHa	54.211	4.760
142AspCb	142AspHba	41.434	2.804
142AspCb	142AspHbb	41.434	2.989
143AspCa	143AspHa	52.951	5.095
143AspCb	143AspHba	43.871	2.723
143AspCb	143AspHbb	43.863	2.922
144GluCa	144GluHa	54.119	4.517
144GluCb	144GluHba	30.578	2.414
144GluCg	144GluHga	36.083	2.413
145GlnCa	145GlnHa	56.255	5.200
145GlnCb	145GlnHba	30.592	2.354
145GlnCg	145GlnHga	34.138	2.315
145GlnCg	145GlnHgb	34.135	2.459
146TyrCa	146TyrHa	58.617	5.114
147IleCa	147IleHa	60.128	5.148
147IleCa	147IleHa	60.131	5.200
147IleCb	147IleHb	41.815	1.848
147IleCd1	147IleHd1*	14.708	0.819
147IleCg1	147IleHg1a	28.767	1.799

147IleCg2	147IleHg2*	17.768	0.974
148TrpCa	148TrpHa	55.671	6.017
149GluCa	149GluHa	54.986	5.745
149GluCb	149GluHba	32.525	2.163
149GluCg	149GluHga	36.391	2.176
150SerCa	150SerHa	57.997	4.840
150SerCb	150SerHbb	67.387	3.827
150SerCb	150SerHba	67.698	3.795
151AsnCa	151AsnHa	52.051	5.385
151AsnCb	151AsnHbb	38.272	2.862
151AsnCb	151AsnHba	38.273	2.833
152AlaCb	152AlaHb*	16.277	1.181
153GlyCa	153GlyHab	44.745	4.351
153GlyCa	153GlyHaa	44.735	4.325
154GlyCa	154GlyHab	46.125	4.268
154GlyCa	154GlyHaa	46.091	3.838
155SerCa	155SerHa	56.492	5.469
155SerCb	155SerHba	66.619	3.675
155SerCb	155SerHba	66.665	3.732
156PheCa	156PheHa	54.832	5.270
157ThrCa	157ThrHa	58.844	5.685
157ThrCb	157ThrHb	72.500	4.006
157ThrCg2	157ThrHg2*	20.736	1.148
158ValCa	158ValHa	61.497	5.604
158ValCb	158ValHb	34.968	2.174
158ValCga	158ValHga*	22.074	1.129
158ValCgb	158ValHgb*	22.660	1.341
159ThrCa	159ThrHa	61.340	5.110
159ThrCb	159ThrHb	72.189	3.907
159ThrCg2	159ThrHg2*	20.273	1.426
160LeuCa	160LeuHa	56.595	3.785
160LeuCb	160LeuHba	40.993	1.258
160LeuCb	160LeuHbb	40.966	1.355
160LeuCda	160LeuHda*	22.822	0.620
160LeuCdb	160LeuHdb*	24.759	0.958
160LeuCg	160LeuHg	27.127	1.323
161AspCa	161AspHa	54.133	4.498
161AspCb	161AspHba	41.949	2.810
162GluCa	162GluHa	54.962	4.774
162GluCb	162GluHba	30.079	2.375
162GluCg	162GluHga	36.590	2.115
163ValCa	163ValHa	62.375	4.525
163ValCb	163ValHb	34.686	2.035
163ValCga	163ValHgb*	18.646	0.903
163ValCgb	163ValHga*	20.537	0.899

164AsnCa	164AsnHa	53.780	4.880
164AsnCb	164AsnHba	38.873	2.646
165GluCa	165GluHa	56.410	4.171
165GluCb	165GluHba	28.634	2.009
165GluCb	165GluHbb	28.631	2.081
165GluCg	165GluHga	35.579	2.230
166ArgCa	166ArgHa	54.554	4.455
166ArgCb	166ArgHba	30.355	1.852
166ArgCd	166ArgHdb	42.287	3.321
166ArgCd	166ArgHda	42.268	3.038
166ArgCg	166ArgHga	27.196	1.717
167?IleCD1[1491]	167?IleHD1*[1492]	12.818	0.580
167IleCa	167IleHa	60.147	4.194
167IleCb	167IleHb	39.391	1.661
167IleCd1	167IleHd1*	13.485	0.603
167IleCg1	167IleHg1a	25.765	1.282
167IleCg2	167IleHg2*	17.577	0.720
169ArgCa	169ArgHa	56.579	4.720
169ArgCb	169ArgHba	30.348	1.923
169ArgCd	169ArgHda	43.181	3.318
169ArgCg	169ArgHga	26.553	1.711
170GlyCa	170GlyHaa	43.340	3.961
171ThrCa	171ThrHa	61.579	5.416
171ThrCb	171ThrHb	72.628	4.148
171ThrCg2	171ThrHg2*	22.421	1.037
172IleCa	172IleHa	61.233	4.568
172IleCb	172IleHb	40.927	1.854
172IleCd1	172IleHd1*	13.422	0.839
172IleCg1	172IleHg1b	27.954	1.529
172IleCg1	172IleHg1a	27.941	1.074
172IleCg2	172IleHg2*	16.516	0.787
173LeuCa	173LeuHa	53.410	4.959
173LeuCb	173LeuHba	41.796	1.768
173LeuCda	173LeuHda*	26.154	1.042
173LeuCg	173LeuHg	28.878	1.857
174ArgCb	174ArgHba	30.829	1.897
174ArgCd	174ArgHdb	42.280	3.394
174ArgCd	174ArgHda	42.285	3.195
174ArgCg	174ArgHga	25.697	1.659
175LeuCa	175LeuHa	54.536	4.503
175LeuCb	175LeuHba	42.182	1.745
175LeuCda	175LeuHda*	26.081	0.674
175LeuCdb	175LeuHdb*	25.215	0.809
175LeuCg	175LeuHg	28.001	1.610
176PheCa	176PheHa	57.064	4.619

176PheCb	176PheHbb	36.269	3.290
176PheCb	176PheHba	36.266	3.230
177LeuCdb	177LeuHda*	21.763	0.684
177LeuCdb	177LeuHdb*	26.520	0.881
177Leu[2418]	177LeuHa	56.099	4.401
178LysCa	178LysHa	56.151	4.327
178LysCe	178LysHea	41.560	2.926
178LysCe	178LysHeb	41.546	3.045
179AspCa	179AspHa	56.994	4.398
179AspCb	179AspHba	40.274	2.725
180AspCa	180AspHa	52.948	4.887
180AspCb	180AspHbb	39.283	3.102
180AspCb	180AspHba	39.284	2.702
181GlnCa	181GlnHa	53.641	5.024
181GlnCb	181GlnHbb	27.377	2.435
181GlnCb	181GlnHba	27.369	2.260
181GlnCg	181GlnHga	32.179	2.406
182LeuCa	182LeuHa	55.965	4.124
182LeuCb	182LeuHba	38.258	1.928
182LeuCda	182LeuHda*	21.963	0.792
182LeuCdb	182LeuHdb*	25.174	1.066
182LeuCg	182LeuHg	29.092	1.985
183GluCa	183GluHa	57.971	4.233
183GluCb	183GluHba	27.872	2.132
183GluCg	183GluHgb	35.695	2.475
183GluCg	183GluHga	35.705	2.334
184TyrCa	184TyrHa	60.039	4.254
184TyrCb	184TyrHba	36.621	2.686
185LeuCa	185LeuHa	53.727	4.442
185LeuCb	185LeuHba	41.690	1.536
185LeuCdb	185LeuHda*	24.185	0.691
185LeuCdb	185LeuHdb*	25.224	0.800
185LeuCg	185LeuHg	27.749	1.067
186GluCa	186GluHa	55.011	4.373
186GluCb	186GluHba	29.060	2.261
186GluCg	186GluHgb	35.683	2.441
186GluCg	186GluHga	35.691	2.293
187GluCa	187GluHa	60.053	4.767
187GluCb	187GluHba	28.906	2.096
187GluCg	187GluHgb	37.529	2.436
187GluCg	187GluHga	37.525	2.381
188LysCa	188LysHa	59.648	3.974
188LysCb	188LysHbb	31.770	1.959
188LysCb	188LysHba	31.766	1.822
188LysCd	188LysHdb	28.897	1.745

188LysCd	188LysHda	28.891	1.708
188LysCe	188LysHea	41.524	3.028
188LysCg	188LysHga	24.331	1.416
188LysCg	188LysHgb	24.322	1.533
189ArgCa	189ArgHa	56.899	4.252
189ArgCb	189ArgHba	29.071	2.036
189ArgCd	189ArgHda	41.231	3.237
189ArgCg	189ArgHga	24.360	1.550
190IleCa	190IleHa	65.592	3.511
190IleCb	190IleHb	37.664	1.948
190IleCd1	190IleHd1*	12.845	0.938
190IleCg1	190IleHg1a	28.944	1.095
190IleCg2	190IleHg2*	18.501	0.974
191LysCa	191LysHa	60.493	3.847
191LysCb	191LysHbb	31.754	1.909
191LysCb	191LysHba	31.759	1.855
191LysCd	191LysHdb	29.063	1.973
191LysCd	191LysHda	29.029	1.708
191LysCe	191LysHea	41.595	2.988
191LysCg	191LysHga	26.532	1.730
192GluCa	192GluHa	59.002	4.086
192GluCb	192GluHbb	29.090	2.344
192GluCb	192GluHba	29.084	1.570
192GluCg	192GluHga	36.130	2.251
192GluCg	192GluHgb	36.131	2.491
193ValCa	193ValHa	65.151	3.862
193ValCb	193ValHb	31.318	2.325
193ValCga	193ValHga*	20.123	0.675
193ValCgb	193ValHgb*	21.897	0.902
194IleCa	194IleHa	64.949	3.655
194IleCb	194IleHb	37.043	1.900
194IleCd1	194IleHd1*	13.552	0.825
194IleCg2	194IleHg2*	16.915	0.855
195LysCa	195LysHa	58.304	4.001
195LysCb	195LysHba	30.841	1.890
195LysCb	195LysHbb	30.856	2.051
195LysCd	195LysHda	28.218	1.746
195LysCe	195LysHea	41.810	2.997
195LysCg	195LysHga	24.284	1.465
196ArgCa	196ArgHa	58.274	4.022
196ArgCb	196ArgHba	30.508	1.505
196ArgCd	196ArgHdb	43.053	3.171
196ArgCd	196ArgHda	43.050	3.126
196ArgCg	196ArgHga	26.674	1.512
197HisCa	197HisHa	57.117	4.954

197HisCb	197HisHba	33.567	3.035
197HisCb	197HisHba	33.441	2.953
198SerCa	198SerHa	58.009	4.769
198SerCb	198SerHbb	63.666	4.123
198SerCb	198SerHba	63.726	3.747
198SerCb	198SerHba	63.680	3.728
199GluCa	199GluHa	58.352	3.878
199GluCb	199GluHba	29.043	1.604
199GluCb	199GluHbb	29.015	1.719
199GluCg	199GluHgb	35.585	1.921
199GluCg	199GluHga	35.588	1.688
200PheCa	200PheHa	56.579	4.709
200PheCb	200PheHba	37.747	2.956
200PheCb	200PheHbb	37.770	3.333
201ValCa	201ValHa	62.732	4.034
201ValCb	201ValHb	31.996	2.130
201ValCgb	201ValHgb*	20.392	1.145
201ValCgb	201ValHga*	21.689	0.981
202AlaCa	202AlaHa	52.632	4.152
202AlaCb	202AlaHb*	18.332	1.130
203TyrCa	203TyrHa	55.408	4.764
203TyrCb	203TyrHba	39.948	3.004
205IleCa	205IleHa	60.093	4.738
205IleCb	205IleHb	38.042	1.774
205IleCd1	205IleHd1*	13.633	0.938
205IleCg1	205IleHg1a	27.156	1.580
205IleCg2	205IleHg2*	16.575	0.752
206GlnCb	206GlnHbb	29.173	2.353
206GlnCb	206GlnHba	29.131	2.262
206GlnCg	206GlnHga	35.740	2.348
206GlnCg	206GlnHgb	35.745	2.552
207LeuCa	207LeuHa	56.661	4.754
207LeuCb	207LeuHbb	44.515	1.766
207LeuCb	207LeuHba	44.523	1.563
207LeuCda	207LeuHda*	25.817	0.943
207LeuCdb	207LeuHdb*	24.745	0.949
207LeuCg	207LeuHg	27.718	1.753
{743}[1755]	(160Leu/{743})(Hdb*/[1756])	25.079	0.960
(7Glu/174Arg)([1904]/Cb)	174Arg[1907]	30.845	2.036
({1001}/91Asn)([2282]/Cb)	({1001}/91Asn)([2283]/Hbb)	38.884	2.729
({1241}/30Phe)([2769]/Ca)	({1241}/30Phe)([2770]/Ha)	59.215	4.480

Appendix B

Below is a summary table of the side-chain assignments of the N-terminal domain bound to ADP

Hsp90 N-terminal domain - ADP state		Chemical Shift	
Carbon Assignment	Proton Assignment	C(ppm)	H(ppm)
1MetCa	1MetHa	54.77113	4.50893
1MetCb	1MetHb*	32.5107	2.1066
1MetCg	1MetHgb	31.63078	2.59662
1MetCg	1MetHga	31.62461	2.5417
3SerCa	3SerHa	57.45169	4.89937
3SerCb	3SerHbb	64.06878	3.68558
3SerCb	3SerHba	64.06766	3.67099
4GluCa	4GluHa	55.01642	4.46991
4GluCb	4GluHba	33.86113	1.8717
4GluCb	4GluHbb	33.86984	1.91354
4GluCg	4GluHga	36.51065	2.21466
4GluCg	4GluHgb	36.515	2.26608
5ThrCa	5ThrHa	61.17092	4.72018
5ThrCb	5ThrHb	69.52271	3.59221
5ThrCg2	5ThrHg2*	20.74114	0.92646
7GluCa	7GluHa	54.77219	4.5948
7GluCb	7GluHbb	30.57878	2.35094
7GluCb	7GluHba	30.59556	2.07402
7GluCg	7GluHga	36.87051	2.05684
7GluCg	7GluHgb	36.86937	2.24495
8PheCa	8PheHa	59.04794	4.5578
8PheCb	8PheHb*	40.29741	2.91815
11GluCa	11GluHa	59.48966	4.11678
11GluCb	11GluHbb	28.70644	2.04467

11GluCb	11GluHba	28.68901	1.95359
11GluCg	11GluHga	37.70086	2.307
11GluCg	11GluHgb	37.69214	2.32857
12IleCa	12IleHa	63.35218	3.5307
12IleCb	12IleHb	36.5124	2.24023
12IleCd1	12IleHd1*	10.88951	0.91013
12IleCg1	12IleHg1a	28.18809	1.14527
12IleCg1	12IleHg1b	28.13589	1.80594
12IleCg2	12IleHg2*	17.78137	0.43907
13ThrCa	13ThrHa	66.35808	3.6292
13ThrCb	13ThrHb	67.42186	4.23469
13ThrCg2	13ThrHg2*	23.90661	1.14208
14GlnCa	14GlnHa	58.3023	3.98023
14GlnCb	14GlnHbb	27.3249	2.08139
14GlnCb	14GlnHba	27.31293	2.06134
14GlnCg	14GlnHgb	33.18425	2.49216
14GlnCg	14GlnHga	33.18425	2.36732
15LeuCa	15LeuHa	57.63956	4.05058
15LeuCda	15LeuHda*	25.95763	0.87754
15LeuCg	15LeuHg	25.21405	1.49395
17SerCa	17SerHa	61.05374	4.09421
17SerCb	17SerHbb	62.1713	3.93088
17SerCb	17SerHba	62.17534	3.89653
18LeuCa	18LeuHa	57.43649	4.14968
18LeuCb	18LeuHb*	41.93146	1.80641
18LeuCda	18LeuHdb*	24.67067	0.80519
18LeuCda	18LeuHda*	23.09799	0.48038
18LeuCg	18LeuHg	26.6601	1.62466
19IleCa	19IleHa	64.01425	3.73676
19IleCd1	19IleHd1*	12.63857	0.747
19IleCg1	19IleHg1*	28.23656	1.61264
19IleCg2	19IleHg2*	17.73245	0.92533
20IleCa	20IleHa	64.87412	3.57676

20IleCb	20IleHb	37.45314	1.81251
20IleCd1	20IleHd1*	13.75609	0.84238
20IleCg1	20IleHg1*	29.08446	1.34041
20IleCg2	20IleHg2*	16.76148	0.96384
21AsnCa	26AsnHa	53.83912	4.87504
21AsnCb	21AsnHba	40.12953	2.75982
21AsnCb	21AsnHbb	40.12953	2.86893
27LysCa	27LysHa	59.32596	3.94205
27LysCb	27LysHbb	31.74919	1.91192
27LysCb	27LysHba	31.75303	1.80277
27LysCd	27LysHd*	28.8378	1.68781
27LysCe	27LysHe*	41.42645	2.99898
27LysCg	27LysHga	24.3784	1.39452
27LysCg	27LysHgb	24.38563	1.51376
28GluCa	28GluHa	58.0766	4.09071
28GluCg	28GluHg*	34.30719	1.85518
29IleCa	29IleHa	61.46935	3.45676
29IleCb	29IleHb	37.71916	2.0275
29IleCd1	29IleHd1*	14.50619	0.71099
29IleCg1	29IleHg1a	25.98003	1.2565
29IleCg1	29IleHg1b	26.01982	1.28568
29IleCg2	29IleHg2*	18.98298	0.81147
30PheCa	30PheHa	58.90627	4.43996
30PheCb	30PheHb*	37.33892	2.57658
31LeuCa	31LeuHa	56.38285	3.07669
31LeuCb	31LeuHba	40.34149	0.30161
31LeuCb	31LeuHbb	40.34149	1.15681
31LeuCda	31LeuHdb*	23.52633	0.69607
31LeuCdb	31LeuHda*	25.04905	0.67772
31LeuCg	31LeuHg	26.16148	1.0603
32ArgCa	32ArgHa	58.05639	3.63575
32ArgCb	32ArgHb*	28.21918	1.70412
32ArgCd	32ArgHda	43.12601	3.00439

32ArgCd	32ArgHdb	43.10491	3.03545
32ArgCg	32ArgHg*	24.73468	1.38443
33GluCa	33GluHa	56.13252	4.18269
33GluCb	33GluHba	28.87386	1.95779
33GluCg	33GluHga	35.33032	2.1342
33GluCg	33GluHgb	35.3338	2.18056
34LeuCa	34LeuHa	57.07705	4.22507
34LeuCd*	34LeuHd*	26.26253	0.92215
35IleCa	35IleHa	64.80614	3.65328
35IleCb	35IleHb	36.41004	1.99189
35IleCd1	35IleHd1*	12.75071	0.72606
35IleCg2	35IleHg2*	17.21623	0.91249
36SerCa	36SerHa	60.7591	4.23709
36SerCb	36SerHb*	62.22978	3.98174
37AsnCa	37AsnHa	54.13134	4.22942
37AsnCb	37AsnHb*	37.23693	3.05404
38AlaCa	38AlaHa	54.3296	4.10235
38AlaCb	38AlaHb*	18.41595	1.51781
39SerCa	39SerHa	61.07525	3.97921
39SerCb	39SerHb*	62.20654	4.00749
40AspCa	40AspHa	56.74101	4.37748
40AspCb	40AspHbb	40.19435	2.80231
40AspCb	40AspHba	40.19726	2.70024
41AlaCa	41AlaHa	54.20045	4.13886
41AlaCb	41AlaHb*	18.36008	1.62189
42LeuCa	42LeuHa	57.10168	3.8397
42LeuCda	42LeuHdb*	24.4681	0.42017
42LeuCdb	42LeuHda*	25.01955	0.05401
42LeuCg	42LeuHg	26.51948	1.23355
43AspCa	43AspHa	57.30427	4.26884
43AspCb	43AspHb*	39.21463	2.65712
44LysCa	44LysHa	60.11309	4.08563
44LysCb	44LysHbb	32.48183	2.04346

44LysCb	44LysHba	32.47746	1.86513
44LysCd	44LysHd*	29.02865	1.65369
44LysCe	44LysHe*	41.62879	2.93219
44LysCg	44LysHg*	24.73923	1.48786
45IleCa	45IleHa	59.58801	4.49818
45IleCb	45IleHb	38.2589	1.45491
45IleCd1	45IleHd1*	14.2315	1.00629
45IleCg1	45IleHg1*	28.94356	1.24427
45IleCg2	45IleHg2*	20.00142	1.27944
46ArgCa	46ArgHa	59.59079	3.89675
46ArgCb	46ArgHbb	29.40674	1.87864
46ArgCb	46ArgHba	29.40165	1.76639
46ArgCd	46ArgHda	43.4025	3.25278
46ArgCd	46ArgHdb	43.39665	3.41019
46ArgCg	46ArgHgb	26.51912	1.54181
46ArgCg	46ArgHga	26.52496	1.38585
47TyrCa	47TyrHa	60.61557	4.3291
47TyrCb	47TyrHbb	37.20562	3.1766
47TyrCb	47TyrHba	37.20207	3.10915
48LysCa	48LysHa	58.86602	4.0278
48LysCb	48LysHba	32.4235	1.88188
48LysCb	48LysHbb	32.42361	2.03951
48LysCd	48LysHda	29.08312	1.3977
48LysCd	48LysHdb	29.09857	1.49974
48LysCe	48LysHe*	41.30372	2.99705
48LysCg	48LysHga	25.21047	1.50797
48LysCg	48LysHgb	25.20973	1.71796
49SerCa	49SerHa	59.74597	4.37299
49SerCb	49SerHba	62.77046	3.86287
50LeuCa	50LeuHa	56.84152	4.13315
50LeuCb	50LeuHba	40.76437	1.46711
50LeuCb	50LeuHbb	40.77284	1.83189
50LeuCda	50LeuHda*	21.7745	0.86413

50LeuCdb	50LeuHdb*	24.8587	0.94141
50LeuCg	50LeuHg	25.78607	2.00999
51SerCa	51SerHa	57.78125	4.61252
51SerCb	51SerHbb	63.30075	3.94882
51SerCb	51SerHba	63.27626	3.85399
52AspCa	52AspHa	51.10865	5.0863
52AspCb	52AspHbb	40.89652	2.82081
52AspCb	52AspHba	40.8318	2.59795
54LysCa	54LysHa	58.03698	3.94444
54LysCb	54LysHba	30.82419	1.84171
54LysCb	54LysHbb	30.82965	1.99375
54LysCd	54LysHd*	28.31953	1.52933
54LysCe	54LysHe*	41.19594	3.01262
54LysCg	54LysHga	24.3498	1.43202
54LysCg	54LysHgb	24.34789	1.50405
55GlnCa	55GlnHa	56.68185	3.77645
55GlnCb	55GlnHba	26.97492	1.76452
55GlnCb	55GlnHbb	26.97152	1.79888
55GlnCg	55GlnHga	32.95509	2.19891
55GlnCg	55GlnHgb	32.94148	2.66273
56LeuCa	56LeuHa	54.40758	4.26091
56LeuCb	56LeuHba	42.21262	1.72303
56LeuCb	56LeuHbb	42.21601	1.78075
56LeuCda	56LeuHda*	23.30617	0.85953
56LeuCdb	56LeuHdb*	24.39721	1.01006
57GluCa	57GluHa	58.72454	3.87145
57GluCb	57GluHb*	28.87384	1.68437
57GluCg	57GluHg*	36.56271	2.36907
58ThrCa	58ThrHa	61.73638	3.96924
58ThrCb	58ThrHb	68.37347	4.33368
58ThrCg2	58ThrHg2*	22.59536	1.27276
59GluCa	59GluHa	60.2168	3.7967
59GluCb	59GluHbb	29.13628	2.24966

59GluCb	59GluHba	29.15073	2.05058
59GluCg	59GluHgb	36.5747	2.44271
59GluCg	59GluHga	36.5747	2.35299
62LeuCa	62LeuHa	53.16432	4.23485
62LeuCb	62LeuHba	40.29237	1.18579
62LeuCd*	62LeuHd*	23.31653	0.64263
63PheCa	63PheHa	55.8845	5.00325
63PheCb	63PheHb*	41.3097	2.96209
64IleCa	64IleHa	59.81747	4.93677
64IleCb	64IleHb	39.71082	1.78477
64IleCd1	64IleHd1*	14.07301	0.76622
64IleCg2	64IleHg2*	16.20008	0.78474
65ArgCa	65ArgHa	54.18525	5.53854
65ArgCb	65ArgHb*	33.01167	1.64216
65ArgCd	65ArgHda	42.77034	2.44507
65ArgCd	65ArgHdb	42.78151	2.69064
65ArgCg	65ArgHgb	26.49021	1.52666
65ArgCg	65ArgHga	26.49313	1.28017
66IleCa	66IleHa	59.95456	5.06063
66IleCb	66IleHb	38.50376	1.91818
66IleCd1	66IleHd1*	14.0644	0.77851
66IleCg1	66IleHg1*	27.16576	1.59597
66IleCg2	66IleHg2*	17.65167	0.92142
67ThrCa	67ThrHa	58.88494	4.86587
67ThrCb	67ThrHb	70.93075	4.00536
67ThrCg2	67ThrHg2*	20.88052	1.17051
69LysCa	69LysHa	58.57973	4.11159
69LysCb	69LysHb*	31.51625	1.87949
69LysCd	69LysHd*	29.00031	1.54281
69LysCe	69LysHe*	41.42241	2.97709
69LysCg	69LysHg*	24.20047	1.23415
71GluCa	71GluHa	58.59288	4.18876
71GluCb	71GluHbb	27.81552	2.13834

71GluCb	71GluHba	27.81552	2.01487
71GluCg	71GluHga	36.08448	2.31747
71GluCg	71GluHgb	36.09111	2.43765
72GlnCa	72GlnHa	54.78067	4.32885
72GlnCb	72GlnHbb	29.55326	2.24501
72GlnCb	72GlnHba	29.55326	2.1975
72GlnCg	72GlnHgb	35.61215	2.40783
72GlnCg	72GlnHga	35.62801	2.24094
73LysCb	73LysHb*	28.6824	1.75905
73LysCe	73LysHe*	41.42406	3.06539
73LysCg	73LysHg*	25.16843	1.43974
74ValCa	74ValHa	58.41451	5.09997
74ValCb	74ValHb	36.54701	1.43739
74ValCga	74ValHga*	22.23198	0.24593
74ValCgb	74ValHgb*	22.66643	0.50266
75LeuCa	75LeuHa	52.75916	4.71713
75LeuCda	75LeuHda*	22.52352	0.94484
75LeuCg	75LeuHg	25.17623	1.05219
76GluCa	76GluHa	53.80305	5.78705
76GluCb	76GluHb*	31.48585	2.04904
76GluCg	76GluHgb	37.40147	2.20071
76GluCg	76GluHga	37.39126	1.8657
77IleCa	77IleHa	60.61085	4.78717
77IleCb	77IleHb	40.05743	1.84032
77IleCd1	77IleHd1*	15.67288	0.84268
77IleCg2	77IleHg2*	17.49525	0.71014
79AspCa	79AspHa	52.03778	5.64634
79AspCb	79AspHba	46.36274	2.49962
80SerCa	80SerHa	54.27698	5.30088
80SerCb	80SerHb*	61.76143	4.07082
81GlyCa	81GlyHaa	44.51916	4.03111
81GlyCa	81GlyHab	44.51916	4.05362
82IleCa	82IleHa	61.94855	3.83464

82IleCb	82IleHb	39.99568	1.71097
82IleCd1	82IleHd1*	15.44945	0.90635
82IleCg1	82IleHg1*	29.08112	1.41572
82IleCg2	82IleHg2*	15.675	1.3027
84MetCg	84MetHg*	33.38287	2.0572
85ThrCa	85ThrHa	59.81373	4.67327
85ThrCb	85ThrHb	69.76881	4.97031
85ThrCg2	85ThrHg2*	22.02574	1.30353
87AlaCa	87AlaHa	54.1944	3.84984
87AlaCb	87AlaHb*	17.61399	1.2477
88GluCa	88GluHa	58.72424	3.80427
88GluCb	88GluHba	29.22487	2.08259
88GluCb	88GluHbb	29.21737	2.33149
88GluCg	88GluHg*	37.06749	2.40981
90IleCa	90IleHa	64.58153	3.36737
90IleCb	90IleHb	38.77638	1.44078
90IleCd1	90IleHd1*	15.65845	0.55947
90IleCg2	90IleHg2*	16.95458	0.38014
91AsnCa	91AsnHa	55.13812	4.47759
91AsnCb	91AsnHba	38.61943	2.59495
91AsnCb	91AsnHbb	38.61943	2.69223
92AsnCa	92AsnHa	56.85814	4.36433
92AsnCb	92AsnHba	39.88002	2.82218
92AsnCb	92AsnHbb	39.88301	2.86528
93LeuCa	93LeuHa	53.92854	4.23109
93LeuCda	93LeuHda*	19.27377	-0.92644
93LeuCdb	93LeuHdb*	23.85487	-0.93698
93LeuCg	93LeuHg	24.89454	0.57949
94GlyCa	94GlyHab	47.50461	4.28282
94GlyCa	94GlyHaa	47.4737	3.44824
95ThrCa	95ThrHa	63.32792	4.72715
95ThrCb	95ThrHb	69.89895	4.45538
95ThrCg2	95ThrHg2*	21.67281	1.44555

96IleCb	96IleHb	42.225	1.75698
96IleCd1	96IleHd1*	15.15061	0.84352
96IleCg2	96IleHg2*	17.71295	0.94337
101ThrCa	101ThrHa	62.42334	4.4494
101ThrCb	101ThrHb	69.31998	4.19229
101ThrCg2	101ThrHg2*	20.54389	1.10921
103AlaCa	103AlaHa	54.16397	4.15678
103AlaCb	103AlaHb*	17.77203	1.61947
104PheCa	104PheHa	58.31431	4.99537
104PheCb	104PheHba	45.40097	2.63725
105MetCa	105MetHa	59.16603	3.96297
105MetCb	105MetHbb	31.78518	1.9352
105MetCb	105MetHba	31.77292	1.79661
105MetCg	105MetHg*	28.64183	1.53023
106GluCa	106GluHa	58.7075	3.88968
106GluCb	106GluHb*	28.6652	2.06032
106GluCg	106GluHga	36.08073	2.18752
106GluCg	106GluHgb	36.07362	2.38437
107AlaCa	107AlaHa	54.4725	4.10827
107AlaCb	107AlaHb*	16.33778	1.31835
108LeuCa	108LeuHa	57.13081	4.16394
108LeuCb	108LeuHbb	40.80399	1.84501
108LeuCb	108LeuHba	40.78511	1.48465
108LeuCda	108LeuHda*	21.3178	0.84189
108LeuCdb	108LeuHdb*	24.43074	0.96196
109SerCa	109SerHa	60.78479	4.21329
109SerCb	109SerHb*	62.20286	3.96016
110AlaCa	110AlaHa	51.23617	4.5045
110AlaCb	110AlaHb*	18.22106	1.48708
111GlyCa	111GlyHaa	44.77482	3.81043
111GlyCa	111GlyHab	44.80216	4.34918
112AlaCa	112AlaHa	51.78181	4.27634
112AlaCb	112AlaHb*	18.99158	1.24542

113AspCa	113AspHa	53.43276	4.64835
113AspCb	113AspHbb	43.14575	2.77904
113AspCb	113AspHba	43.15456	2.70826
115SerCa	115SerHa	61.05032	4.07936
115SerCb	115SerHb*	62.61406	4.34932
116MetCa	116MetHa	55.84994	4.50662
116MetCb	116MetHb*	31.90764	2.3555
116MetCg	116MetHgb	30.19466	3.15084
116MetCg	116MetHga	30.19945	3.12641
117IleCa	117IleHa	64.69472	2.95784
117IleCb	117IleHb	36.93706	1.89539
117IleCd1	117IleHd1*	15.6483	0.75275
118GlyCa	118GlyHab	46.25155	4.18209
118GlyCa	118GlyHaa	46.24363	3.79831
119GlnCa	119GlnHa	56.15626	4.17059
119GlnCb	119GlnHb*	28.07847	1.86996
119GlnCg	119GlnHgb	33.37055	2.2637
119GlnCg	119GlnHga	33.37285	2.14776
120PheCa	120PheHa	56.95853	4.24773
120PheCb	120PheHba	39.21114	2.70945
120PheCb	120PheHbb	39.22191	3.18343
121GlyCa	121GlyHaa	45.62642	4.12908
121GlyCa	121GlyHab	45.62642	4.14332
122ValCb	122ValHb	31.72217	2.80663
122ValCga	122ValHga*	17.7151	0.54641
122ValCgb	122ValHgb*	22.30748	0.98199
123GlyCa	123GlyHaa	47.50114	3.47161
123GlyCa	123GlyHac	47.48974	4.26127
124PheCa	124PheHa	60.57274	4.75637
124PheCb	124PheHb*	39.89529	2.89815
125TyrCa	125TyrHa	60.56576	3.9198
125TyrCb	125TyrHba	36.94652	2.7783
125TyrCb	125TyrHbb	36.95338	2.82908

126SerCa	126SerHa	61.19523	3.81708
126SerCb	126SerHb*	62.6921	3.94582
127LeuCa	127LeuHa	57.54561	3.85469
127LeuCb	127LeuHb*	40.91418	1.26276
127LeuCda	127LeuHda*	23.44551	0.96256
127LeuCdb	127LeuHdb*	24.26844	1.04641
128PheCa	128PheHa	60.17733	4.85133
128PheCb	128PheHbb	36.84709	3.51225
128PheCb	128PheHba	36.87811	2.88284
129LeuCa	129LeuHa	57.64095	4.2592
129LeuCb	129LeuHba	41.91142	1.69315
129LeuCb	129LeuHbb	41.92947	1.80022
129LeuCd*	129LeuHd*	24.45555	0.84442
130ValCa	130ValHa	59.81857	4.55129
130ValCb	130ValHb	32.43711	2.02061
130ValCga	130ValHga*	14.9016	-0.6205
130ValCgb	130ValHgb*	21.51615	0.43978
131AlaCa	131AlaHa	50.40237	5.05697
131AlaCb	131AlaHb*	21.53992	1.03774
133ArgCa	133ArgHa	54.27309	5.11035
133ArgCb	133ArgHb*	33.00333	1.93411
133ArgCd	133ArgHda	42.77034	2.47297
133ArgCd	133ArgHdb	42.77034	2.72078
133ArgCg	133ArgHga	26.58646	1.51446
133ArgCg	133ArgHgb	26.58646	1.64376
134ValCa	134ValHa	58.42276	5.66134
134ValCb	134ValHb	34.7211	1.93603
134ValCga	134ValHga*	21.80761	0.8339
134ValCgb	134ValHgb*	20.76138	1.23029
136ValCa	136ValHa	61.01956	4.8734
136ValCb	136ValHb	32.3462	2.38207
136ValCga	136ValHga*	20.83107	0.83427
137IleCa	137IleHa	59.49921	5.20592

137IleCb	137IleHb	39.0146	1.88342
137IleCd1	137IleHd1*	14.6683	0.81835
137IleCg2	137IleHg2*	19.11328	0.9675
138SerCa	138SerHa	56.73488	5.5157
138SerCb	138SerHba	66.21504	3.27101
138SerCb	138SerHbb	66.23352	3.8445
140SerCa	140SerHa	54.54077	4.93778
140SerCb	140SerHba	63.01566	3.34184
140SerCb	140SerHbb	63.01069	3.61647
141AsnCa	141AsnHa	54.78676	4.44629
141AsnCb	141AsnHb*	36.86073	2.82268
142AspCa	142AspHa	53.97797	4.72545
142AspCb	142AspHba	41.55015	2.76408
142AspCb	142AspHbb	41.54428	2.96318
143AspCa	143AspHa	52.7606	5.04827
143AspCb	143AspHba	44.73479	2.56315
143AspCb	143AspHbb	44.72598	2.59457
144GluCa	144GluHa	53.86506	4.47701
144GluCb	144GluHb*	30.5646	2.09629
144GluCg	144GluHg*	36.03084	2.41523
145GlnCa	145GlnHa	56.00925	5.15323
145GlnCb	145GlnHb*	29.58914	2.27932
145GlnCg	145GlnHga	34.09523	2.27454
145GlnCg	145GlnHgb	34.09238	2.41878
146TyrCa	146TyrHa	58.31518	5.07394
147IleCa	147IleHa	59.55958	5.16104
147IleCb	147IleHb	42.26524	1.75609
147IleCd1	147IleHd1*	14.65535	0.80424
147IleCg1	147IleHg1*	28.68721	1.75076
147IleCg2	147IleHg2*	17.89912	0.93446
148TrpCa	148TrpHa	55.33588	5.97614
148TrpCb	148TrpHba	34.47832	3.62662
149GluCa	149GluHa	54.90391	5.70488

149GluCb	149GluHb*	32.4936	1.9898
149GluCg	149GluHg*	36.04964	2.14944
150SerCa	150SerHa	57.08361	4.79913
150SerCb	150SerHbb	63.3606	4.11198
150SerCb	150SerHba	63.34828	3.6506
151AsnCa	151AsnHa	51.90289	5.36643
151AsnCb	151AsnHbb	38.20426	2.81832
151AsnCb	151AsnHba	38.20067	2.77198
152AlaCa	152AlaHa	53.14582	3.8354
152AlaCb	152AlaHb*	16.42707	1.20864
153GlyCa	153GlyHab	44.79305	4.38017
153GlyCa	153GlyHaa	44.7657	3.78673
154GlyCa	154GlyHaa	46.26048	3.84226
154GlyCa	154GlyHab	46.25136	4.16769
155SerCa	155SerHa	56.12931	5.31455
155SerCb	155SerHb*	66.34251	3.67478
155SerCb	155SerHb*	66.34867	3.61502
156PheCa	156PheHa	54.68211	5.20494
157ThrCa	157ThrHa	58.46339	5.63915
157ThrCb	157ThrHb	72.05077	3.96648
157ThrCg2	157ThrHg2*	20.83556	1.10765
158ValCa	158ValHa	61.2116	5.55902
158ValCb	158ValHb	34.94537	2.08244
158ValCga	158ValHga*	22.20321	1.0551
158ValCgb	158ValHgb*	22.73896	1.27013
159ThrCa	159ThrHa	61.04279	5.03137
159ThrCb	159ThrHb	71.73457	3.84216
159ThrCg2	159ThrHg2*	20.37287	1.3771
160LeuCa	160LeuHa	56.31722	3.67378
160LeuCb	160LeuHba	40.86294	1.18544
160LeuCda	160LeuHda*	22.89405	0.54895
160LeuCdb	160LeuHdb*	24.81622	0.9175
160LeuCg	160LeuHg	26.50795	1.25585

161AspCa	161AspHa	53.87864	4.4583
161AspCb	161AspHb*	41.66961	2.76504
162GluCa	162GluHa	54.69125	4.72506
162GluCb	162GluHb*	30.06502	2.331
162GluCg	162GluHg*	36.51194	2.06494
163ValCa	163ValHa	62.03311	4.48452
163ValCb	163ValHb	34.65556	1.97989
163ValCga	163ValHgb*	18.83646	0.8483
163ValCgb	163ValHga*	20.58127	0.84613
164AsnCa	164AsnHa	53.52763	4.82044
164AsnCb	164AsnHb*	38.61142	2.62791
165GluCa	165GluHa	56.13378	4.12387
165GluCb	165GluHbb	28.64796	1.94349
165GluCb	165GluHba	28.64974	1.96903
165GluCg	165GluHg*	35.41153	2.15961
166ArgCa	166ArgHa	54.35395	4.42223
166ArgCb	166ArgHb*	30.35769	1.7856
166ArgCd	166ArgHdb	42.71301	3.19384
166ArgCd	166ArgHda	42.70944	3.1449
166ArgCg	166ArgHg*	27.21795	1.63362
167IleCa	167IleHa	59.97015	4.14434
167IleCb	167IleHb	39.3494	1.59963
167IleCd1	167IleHd1*	13.66214	0.5626
167IleCg1	167IleHg1*	25.99926	1.27067
167IleCg2	167IleHg2*	17.68941	0.67571
169ArgCa	169ArgHa	54.3079	4.43814
169ArgCb	169ArgHb*	30.35054	1.85168
169ArgCd	169ArgHd*	42.74867	3.21015
169ArgCg	169ArgHg*	26.59071	1.67061
170GlyCa	170GlyHa*	43.1995	3.92127
171ThrCa	171ThrHa	61.8209	5.36288
171ThrCb	171ThrHb	71.42497	4.18338
171ThrCg2	171ThrHg2*	22.07488	0.74542

172IleCb	172IleHb	41.39471	1.79715
172IleCd1	172IleHd1*	13.59985	0.79943
172IleCg1	172IleHg1b	28.25314	1.51734
172IleCg1	172IleHg1a	28.25314	1.33588
172IleCg2	172IleHg2*	16.74165	0.69535
173LeuCa	173LeuHa	53.16271	4.91857
173LeuCb	173LeuHb*	41.87027	1.65132
173LeuCd*	173LeuHd*	25.63327	0.98599
173LeuCg	173LeuHg	29.23034	1.88019
174ArgCb	174ArgHb*	30.82217	1.85697
174ArgCb	None	30.8377	1.99603
174ArgCd	174ArgHda	43.10779	3.27582
174ArgCd	174ArgHdb	43.09558	3.39792
174ArgCg	174ArgHg*	25.94604	1.41823
175LeuCa	175LeuHa	54.42528	4.46249
175LeuCb	175LeuHb*	41.94368	1.79439
175LeuCda	175LeuHda*	26.12443	0.63388
175LeuCdb	175LeuHdb*	25.40235	0.76803
175LeuCg	175LeuHg	28.01778	1.55773
176PheCa	176PheHa	56.7726	4.62176
177LeuCa	177LeuHa	55.80934	4.35563
177LeuCda	177LeuHda*	21.91446	0.62872
177LeuCdb	177LeuHdb*	26.44847	0.83468
177LeuCg	177LeuHg	29.61755	1.65173
178LysCa	178LysHa	55.87504	4.28716
178LysCb	178LysHba	34.3659	2.18773
178LysCe	178LysHea	41.43874	2.88567
178LysCe	178LysHeb	41.42464	3.00519
179AspCa	179AspHa	56.70866	4.35789
179AspCb	179AspHb*	40.19159	2.69194
180AspCa	180AspHa	52.70777	4.85569
180AspCb	180AspHba	39.19928	2.67803
180AspCb	180AspHbb	39.19341	3.08769

181GlnCa	181GlnHa	53.3698	4.96786
181GlnCb	181GlnHbb	27.71559	1.93924
181GlnCb	181GlnHba	27.71891	1.94904
181GlnCg	181GlnHg*	32.15708	2.36607
182LeuCa	182LeuHa	56.08266	4.06783
182LeuCb	182LeuHb*	38.39235	1.88901
182LeuCda	182LeuHda*	22.32189	0.74388
182LeuCdb	182LeuHdb*	25.22674	1.02648
182LeuCg	182LeuHg	29.10506	1.95925
183GluCa	183GluHa	57.63401	4.1983
183GluCb	183GluHb*	27.88299	2.07744
183GluCg	183GluHga	35.6373	2.27977
183GluCg	183GluHgb	35.63115	2.33144
184TyrCa	184TyrHa	59.68953	4.21641
184TyrCb	184TyrHb*	37.08907	2.64655
185LeuCa	185LeuHa	53.64643	4.3981
185LeuCda	185LeuHda*	24.30052	0.65211
185LeuCdb	185LeuHdb*	25.34951	0.7473
185LeuCg	185LeuHg	27.46568	1.0138
186GluCa	186GluHa	54.77548	4.33509
186GluCb	186GluHb*	29.07116	2.22101
186GluCg	186GluHga	35.6321	2.25337
186GluCg	186GluHgb	35.62461	2.40098
187GluCa	187GluHa	59.72736	4.5018
187GluCb	187GluHb*	29.07158	1.94551
187GluCg	187GluHga	37.68899	2.29653
187GluCg	187GluHgb	37.69883	2.3396
188LysCa	188LysHa	59.33452	3.93364
188LysCb	188LysHba	31.74897	1.78195
188LysCb	188LysHbb	31.75302	1.91866
188LysCd	188LysHdb	28.90995	1.70478
188LysCd	188LysHda	28.90398	1.66796
188LysCe	188LysHe*	41.40337	2.98819

188LysCg	188LysHga	24.39252	1.37614
188LysCg	188LysHgb	24.38357	1.49263
189ArgCa	189ArgHa	56.61791	4.24565
189ArgCb	189ArgHb*	29.08224	1.99594
189ArgCd	189ArgHd*	41.53207	3.17269
189ArgCg	189ArgHg*	24.41907	1.47141
190IleCa	190IleHa	65.40538	3.45757
190IleCb	190IleHb	37.68572	1.89259
190IleCd1	190IleHd1*	13.13746	0.88159
190IleCg1	190IleHg1a	29.09814	1.03181
190IleCg2	190IleHg2*	18.5306	0.92533
191LysCa	191LysHa	60.17138	3.80677
191LysCb	191LysHbb	31.74425	1.92862
191LysCb	191LysHba	31.74425	1.806
191LysCd	191LysHda	29.04081	1.66772
191LysCd	191LysHdb	29.07457	1.93344
191LysCe	191LysHe*	41.47305	2.9484
191LysCg	191LysHg*	26.57018	1.68964
192GluCa	192GluHa	58.65837	4.04875
192GluCb	192GluHba	29.09545	1.52972
192GluCb	192GluHbb	29.09736	2.04451
192GluCg	192GluHgb	36.06788	2.45107
192GluCg	192GluHga	36.06622	2.21114
193ValCa	193ValHa	64.747	3.80452
193ValCb	193ValHb	31.30511	2.28457
193ValCga	193ValHga*	20.22895	0.63463
193ValCgb	193ValHgb*	23.16122	0.85573
194IleCa	194IleHa	64.8701	3.5924
194IleCb	194IleHb	37.01229	1.86913
194IleCd1	194IleHd1*	13.75332	0.78532
194IleCg1	194IleHg1a	28.21175	1.7589
194IleCg2	194IleHg2*	16.96503	0.78705
195LysCa	195LysHa	58.00549	3.96124

195LysCb	195LysHba	30.83318	1.85017
195LysCb	195LysHbb	30.84836	2.01082
195LysCd	195LysHd*	28.22795	1.69156
195LysCe	195LysHe*	41.68641	2.95656
195LysCg	195LysHg*	24.33865	1.41512
196ArgCa	196ArgHa	57.97515	3.98232
196ArgCb	196ArgHb*	30.58074	1.45082
196ArgCd	196ArgHda	42.83205	3.07743
196ArgCd	196ArgHdb	42.82755	3.12019
196ArgCg	196ArgHg*	26.53448	1.21565
197HisCa	197HisHa	56.84624	4.88289
197HisCb	197HisHb*	33.46523	2.78854
198SerCa	198SerHa	57.1253	4.81631
198SerCb	198SerHba	63.32373	3.688
198SerCb	198SerHbb	63.30996	4.08297
199GluCa	199GluHa	58.06307	3.79422
199GluCb	199GluHba	29.04833	1.53883
199GluCb	199GluHbb	29.03122	1.64793
199GluCg	199GluHgb	35.49441	1.8474
199GluCg	199GluHga	35.50327	1.6218
200PheCa	200PheHa	56.23676	4.66642
200PheCb	200PheHbb	37.6083	3.28467
200PheCb	200PheHba	37.61227	2.91199
201ValCa	201ValHa	62.70112	3.93454
201ValCb	201ValHb	31.83034	2.06303
201ValCga	201ValHgb*	20.49271	1.08999
201ValCgb	201ValHga*	21.94792	0.95171
202AlaCa	202AlaHa	52.32129	4.1223
202AlaCb	202AlaHb*	18.41983	1.07383
203TyrCa	203TyrHa	55.18031	4.70635
203TyrCb	203TyrHb*	39.85441	2.92308
205IleCa	205IleHa	59.76362	4.68396
205IleCb	205IleHb	37.86412	1.73321

205IleCd1	205IleHd1*	13.6578	0.88496
205IleCg1	205IleHg1*	27.17359	1.5596
205IleCg2	205IleHg2*	17.0722	0.76427
206GlnCa	206GlnHa	58.70684	3.76651
206GlnCb	206GlnHbb	29.18379	2.31332
206GlnCb	206GlnHba	29.14194	2.2222
206GlnCg	206GlnHgb	35.68546	2.51234
206GlnCg	206GlnHga	35.68065	2.30823
207LeuCa	207LeuHa	56.40499	4.72219
207LeuCb	207LeuHbb	44.36781	1.71569
207LeuCb	207LeuHba	44.37339	1.51897
207LeuCda	207LeuHdb*	24.80197	0.90889
207LeuCdb	207LeuHda*	25.86276	0.90336
207LeuCg	207LeuHg	27.7554	1.69674

Appendix C

Below is a summary table of the side-chain assignments of the N-terminal domain bound to AMPPNP

Hsp90 N-terminal domain - AMPPNP state		Chemical Shift	
Carbon Assignment	Proton Assignment	C(ppm)	H(ppm)
1MetCa	1MetHa	54.77421	4.52068
1MetCb	1MetHb*	32.14673	2.11901
1MetCg	1MetHgb	31.63521	2.60884
1MetCg	1MetHga	31.63386	2.55599
3SerCa	3SerHa	57.42065	4.92628
3SerCb	3SerHba	64.06308	3.67368
3SerCb	3SerHbb	64.06593	3.69234
4GluCa	4GluHa	55.15195	4.47601
4GluCb	4GluHbb	33.86523	1.91469
4GluCb	4GluHba	33.86137	1.85985
4GluCg	4GluHga	36.4055	2.24219
4GluCg	4GluHgb	36.42481	2.26459
5ThrCa	5ThrHa	61.16199	4.71846
5ThrCb	5ThrHb	69.52768	3.60993
5ThrCg2	5ThrHg2*	20.75979	0.94223
7GluCa	7GluHa	54.81386	4.62535
7GluCb	7GluHba	30.53837	2.07445
7GluCb	7GluHbb	30.55313	2.34458
7GluCg	7GluHga	36.83544	2.07542
7GluCg	7GluHgb	36.86937	2.24495
8PheCa	8PheHa	58.99252	4.59589
8PheCb	8PheHb*	39.8828	2.89991
9GlnCa	9GlnHa	56.85349	4.20757
11GluCa	11GluHa	59.60767	4.10628
11GluCg	11GluHga	37.51938	2.31836

11GluCg	11GluHgb	37.51878	2.3594
12IleCa	12IleHa	63.30991	3.54806
12IleCb	12IleHb	35.59231	2.22018
12IleCd1	12IleHd1*	11.15487	0.88964
12IleCg1	12IleHg1a	28.34618	1.11269
12IleCg1	12IleHg1b	28.31328	1.75365
12IleCg2	12IleHg2*	17.64053	0.3998
13ThrCa	13ThrHa	66.25981	3.73993
13ThrCb	13ThrHb	67.48225	4.22962
13ThrCg2	13ThrHg2*	23.62964	1.1901
14GlnCa	14GlnHa	58.32559	3.98257
14GlnCb	14GlnHba	27.3162	2.06738
14GlnCb	14GlnHbb	27.31058	2.082
14GlnCg	14GlnHgb	33.13881	2.48236
14GlnCg	14GlnHga	33.14443	2.36427
15LeuCa	15LeuHa	58.23747	3.997
15LeuCd*	15LeuHd*	25.96183	0.82547
15LeuCg	15LeuHg	25.17719	1.51742
17SerCa	17SerHa	61.00289	4.11179
17SerCb	17SerHba	62.21661	3.92171
17SerCb	17SerHbb	62.21912	3.93953
18LeuCa	18LeuHa	57.41057	4.1335
18LeuCb	18LeuHb*	41.84995	1.84308
18LeuCd*	18LeuHd*	24.43316	0.81984
18LeuCg	18LeuHg	26.53126	1.6182
18LeuCg	18LeuHg	26.80771	1.63482
19IleCa	19IleHa	64.06366	3.67739
19IleCb	19IleHb	36.48421	1.99823
19IleCd1	19IleHd1*	12.86949	0.7728
19IleCg1	19IleHg1a	28.24136	1.18709
19IleCg1	19IleHg1b	28.25418	1.62543
19IleCg2	19IleHg2*	17.73245	0.92533
20IleCa	20IleHa	63.81533	3.9472

20IleCb	20IleHb	37.41656	1.85141
20IleCd1	20IleHd1*	13.74841	0.88071
20IleCg1	20IleHg1*	29.08164	1.40234
20IleCg2	20IleHg2*	16.70821	0.97874
21AsnCa	21AsnHa	53.36743	4.88948
21AsnCb	21AsnHbb	39.87688	2.87458
21AsnCb	21AsnHba	39.88044	2.79734
22ThrCa	22ThrHa	59.26627	4.31239
23?ValCG2|CG1[3058]	None	25.8401	0.36812
27LysCa	27LysHa	59.35667	3.9485
27LysCb	27LysHba	31.75303	1.80277
27LysCb	27LysHbb	31.75058	1.93249
27LysCd	27LysHd*	28.92523	1.68805
27LysCe	27LysHe*	41.42645	2.99898
27LysCg	27LysHgb	24.38563	1.51376
27LysCg	27LysHga	24.38167	1.41654
28GluCa	28GluHa	58.08987	4.0958
28GluCg	28GluHg*	34.5806	1.88967
29IleCa	29IleHa	61.98069	3.48259
29IleCb	29IleHb	37.54029	2.04198
29IleCd1	29IleHd1*	14.57559	0.76133
29IleCg1	29IleHg1b	25.98452	1.3435
29IleCg1	29IleHg1a	25.98452	1.27029
29IleCg2	29IleHg2*	19.74209	0.83193
30PheCa	30PheHa	58.93038	4.41255
30PheCb	30PheHb*	37.33818	2.57097
31LeuCa	31LeuHa	56.39471	3.08661
31LeuCb	31LeuHba	40.33591	0.32263
31LeuCb	31LeuHbb	40.38219	1.15569
31LeuCda	31LeuHda*	25.00528	0.68048
31LeuCdb	31LeuHdb*	23.50714	0.70089
32ArgCa	32ArgHa	58.14693	3.64498
32ArgCb	32ArgHb*	28.20815	1.77094

32ArgCd	32ArgHda	43.12601	3.00439
32ArgCd	32ArgHdb	43.1266	3.01246
32ArgCg	32ArgHg*	25.20971	1.41541
33GluCa	33GluHa	57.20481	3.93449
33GluCb	33GluHba	27.84475	2.06693
33GluCb	33GluHbb	27.84681	2.11418
33GluCg	33GluHgb	35.31964	2.33944
33GluCg	33GluHga	35.32463	2.27361
34LeuCa	34LeuHa	57.2457	4.19245
34LeuCb	34LeuHb*	38.9838	1.85764
34LeuCd*	34LeuHd*	26.27266	0.93887
35IleCa	35IleHa	64.8229	3.6597
35IleCb	35IleHb	36.03373	1.98697
35IleCd1	35IleHd1*	12.74359	0.72299
35IleCg1	35IleHg1a	29.52614	0.97121
35IleCg2	35IleHg2*	17.0361	0.9246
36SerCa	36SerHa	61.40561	4.25191
36SerCb	36SerHb*	61.77988	3.9812
37AsnCa	37AsnHa	54.0623	4.20305
37AsnCb	37AsnHb*	37.3015	3.06977
38AlaCa	38AlaHa	54.34914	4.07224
38AlaCb	38AlaHb*	18.27493	1.49988
39SerCa	39SerHa	61.02609	3.99187
39SerCb	39SerHb*	62.35693	4.02567
40AspCa	40AspHa	56.99114	4.40737
40AspCb	40AspHbb	39.81574	3.19039
40AspCb	40AspHba	39.81574	3.17215
41AlaCa	41AlaHa	54.82643	4.04483
41AlaCb	41AlaHb*	18.23599	1.53241
42LeuCa	42LeuHa	57.36774	3.86088
42LeuCda	42LeuHda*	25.06655	0.06714
42LeuCdb	42LeuHdb*	24.5444	0.42616
42LeuCg	42LeuHg	26.52515	1.09657

43AspCa	43AspHa	57.38491	4.23892
43AspCb	43AspHb*	39.21262	2.67086
44LysCa	44LysHa	59.98187	4.1507
44LysCb	44LysHbb	32.4214	2.05108
44LysCb	44LysHba	32.4214	1.86825
44LysCd	44LysHd*	29.45073	1.65083
44LysCe	44LysHe*	41.58223	2.93979
44LysCg	44LysHg*	25.92197	1.69568
45IleCa	45IleHa	59.56364	4.51287
45IleCb	45IleHb	38.20973	1.45172
45IleCd1	45IleHd1*	14.22522	1.01359
45IleCg1	45IleHg1*	28.94224	1.27937
45IleCg2	45IleHg2*	20.02285	1.28672
46ArgCa	46ArgHa	59.62692	3.90874
46ArgCb	46ArgHba	29.38879	1.77643
46ArgCb	46ArgHbb	29.40044	1.89206
46ArgCd	46ArgHdb	43.38141	3.4138
46ArgCd	46ArgHda	43.3837	3.26109
46ArgCg	46ArgHga	26.51418	1.39195
46ArgCg	46ArgHgb	26.51088	1.55052
47TyrCa	47TyrHa	60.61462	4.33165
47TyrCb	47TyrHbb	37.20094	3.18824
47TyrCb	47TyrHba	37.2044	3.12059
48LysCa	48LysHa	58.89217	4.03645
48LysCb	48LysHbb	32.41744	2.07983
48LysCb	48LysHba	32.42116	1.88247
48LysCd	48LysHda	29.08739	1.72405
48LysCd	48LysHdb	29.08111	1.55515
48LysCe	48LysHe*	41.30372	2.99705
48LysCg	48LysHga	25.17016	1.52666
48LysCg	48LysHgb	25.16178	1.72567
49SerCa	49SerHa	59.66032	4.36696
50LeuCa	50LeuHa	56.83347	4.13335

50LeuCb	50LeuHba	40.78462	1.48426
50LeuCb	50LeuHbb	40.78462	1.83351
50LeuCda	50LeuHda*	21.76815	0.86439
50LeuCdb	50LeuHdb*	24.85974	0.94926
50LeuCg	50LeuHg	25.77028	2.0166
51SerCa	51SerHa	57.84092	4.61324
51SerCb	51SerHbb	63.29645	3.95396
51SerCb	51SerHba	63.29306	3.86899
52AspCa	52AspHa	51.14151	5.09038
52AspCb	52AspHba	40.82912	2.61881
52AspCb	52AspHbb	40.83165	2.81259
54LysCa	54LysHa	58.08131	4.10219
54LysCb	54LysHbb	30.82887	2.01432
54LysCb	54LysHba	30.82673	1.86373
54LysCd	54LysHd*	28.23896	1.69818
54LysCe	54LysHe*	41.19594	3.01262
54LysCg	54LysHgb	24.42696	1.50444
54LysCg	54LysHga	24.42052	1.43194
55GlnCa	55GlnHa	56.69632	3.78819
55GlnCb	55GlnHbb	27.34431	2.25761
55GlnCb	55GlnHba	27.34431	2.24074
55GlnCg	55GlnHga	32.93497	2.22781
55GlnCg	55GlnHgb	32.92448	2.6385
56LeuCa	56LeuHa	54.65311	4.27821
56LeuCb	56LeuHb*	42.25638	1.79182
56LeuCb	56LeuHb*	42.25966	1.74132
56LeuCda	56LeuHda*	23.28649	0.86625
56LeuCdb	56LeuHdb*	24.40049	1.01875
57GluCa	57GluHa	58.75766	3.87571
57GluCb	57GluHb*	28.87384	1.68437
57GluCg	57GluHg*	36.55187	2.37657
58ThrCa	58ThrHa	61.79245	3.94032
58ThrCb	58ThrHb	68.38107	4.33751

58ThrCg2	58ThrHg2*	22.60189	1.27766
59GluCb	59GluHbb	29.13628	2.24966
59GluCb	59GluHba	29.15073	2.05058
59GluCg	59GluHga	37.75194	2.02021
59GluCg	59GluHgb	37.75634	2.04221
62LeuCa	62LeuHa	53.18691	4.23549
62LeuCd*	62LeuHd*	23.35306	0.65139
63PheCa	63PheHa	55.80053	5.00946
63PheCb	63PheHb*	41.43868	2.90612
64IleCa	64IleHa	59.69721	4.9565
64IleCb	64IleHb	39.72377	1.8039
64IleCd1	64IleHd1*	14.05271	0.78516
64IleCg1	64IleHg1a	28.68038	1.75803
64IleCg2	64IleHg2*	16.14739	0.79717
65ArgCa	65ArgHa	54.08449	5.5607
65ArgCb	65ArgHb*	32.93038	1.64587
65ArgCd	65ArgHdb	42.71746	3.23818
65ArgCd	65ArgHda	42.72076	3.21807
65ArgCg	65ArgHg*	26.58628	1.67938
66IleCa	66IleHa	59.89411	5.07809
66IleCb	66IleHb	38.96798	1.88534
66IleCd1	66IleHd1*	14.0644	0.77851
66IleCg1	66IleHg1*	27.18657	1.58467
66IleCg2	66IleHg2*	17.67774	0.93447
67ThrCa	67ThrHa	58.88657	4.87418
67ThrCb	67ThrHb	70.96063	4.01233
67ThrCg2	67ThrHg2*	20.88767	1.17616
69LysCa	69LysHa	52.91777	5.00793
69LysCb	69LysHb*	31.49329	1.88654
69LysCd	69LysHd*	29.06341	1.5686
69LysCe	69LysHe*	41.42241	2.97709
69LysCg	69LysHg*	24.11741	1.256
71GluCa	71GluHa	58.59922	4.19922

71GluCb	71GluHba	27.77854	1.97701
71GluCb	71GluHbb	27.80388	2.10437
71GluCg	71GluHga	36.06825	2.32108
71GluCg	71GluHgb	36.09111	2.43765
72GlnCa	72GlnHa	54.76454	4.47411
72GlnCb	72GlnHbb	29.54829	2.24469
72GlnCb	72GlnHba	29.54829	2.20295
72GlnCg	72GlnHgb	35.61215	2.40783
72GlnCg	72GlnHga	35.62801	2.24094
73LysCa	73LysHa	57.88885	3.52347
73LysCb	73LysHb*	28.67617	1.77169
73LysCe	73LysHe*	41.45974	3.07675
73LysCg	73LysHg*	25.16843	1.43974
74ValCa	74ValHa	58.38681	5.10937
74ValCb	74ValHb	36.55534	1.4509
74ValCga	74ValHga*	22.19022	0.25645
74ValCgb	74ValHgb*	22.62951	0.51172
75LeuCa	75LeuHa	52.76487	4.71642
75LeuCda	75LeuHda*	22.52252	0.95228
75LeuCda	75LeuHdb*	26.95387	1.38571
75LeuCg	75LeuHg	25.15778	1.05944
76GluCa	76GluHa	53.84145	5.78862
76GluCb	76GluHb*	30.47954	2.09364
76GluCg	76GluHgb	37.41271	2.21905
76GluCg	76GluHga	37.40017	1.87985
77IleCa	77IleHa	60.58539	4.74223
77IleCb	77IleHb	40.05335	1.86945
77IleCd1	77IleHd1*	15.57879	0.85535
77IleCg2	77IleHg2*	17.4421	0.72161
79AspCa	79AspHa	52.01229	5.65855
80SerCb	80SerHb*	61.76143	4.07082
81GlyCa	81GlyHaa	44.50716	4.03697
81GlyCa	81GlyHab	44.49582	4.06137

82IleCa	82IleHa	62.33869	3.83283
82IleCb	82IleHb	40.00871	1.71341
82IleCd1	82IleHd1*	15.42764	0.91578
82IleCg1	82IleHg1*	28.70942	1.4639
82IleCg2	82IleHg2*	15.71074	1.3117
84MetCb	84MetHb*	36.86967	2.04737
84MetCg	84MetHg*	33.28854	2.09888
85ThrCa	85ThrHa	59.78731	4.68505
85ThrCb	85ThrHb	69.74801	4.97707
85ThrCg2	85ThrHg2*	21.99138	1.31222
87AlaCa	87AlaHa	54.18846	3.87213
87AlaCb	87AlaHb*	17.62619	1.26554
88GluCa	88GluHa	58.58744	3.80409
88GluCb	88GluHbb	29.21737	2.33149
88GluCb	88GluHba	29.23752	2.09638
88GluCg	88GluHg*	37.46456	2.3785
90IleCa	90IleHa	64.68473	3.36022
90IleCb	90IleHb	38.75383	1.47899
90IleCd1	90IleHd1*	15.53219	0.57901
90IleCg1	90IleHg1*	28.65482	1.74717
90IleCg2	90IleHg2*	16.79903	0.44048
91AsnCa	91AsnHa	55.20162	4.53079
91AsnCb	91AsnHbb	38.79185	2.68467
91AsnCb	91AsnHba	38.77453	2.61705
92AsnCa	92AsnHa	54.69156	4.71773
92AsnCb	92AsnHba	39.83419	2.92803
92AsnCb	92AsnHbb	39.83419	2.97891
93LeuCa	93LeuHa	53.42907	4.18399
93LeuCda	93LeuHda*	19.08773	-0.91503
93LeuCdb	93LeuHdb*	23.55984	-0.97036
93LeuCg	93LeuHg	24.91962	0.60976
95ThrCa	95ThrHa	63.1148	4.79087
95ThrCb	95ThrHb	70.14936	4.41828

95ThrCg2	95ThrHg2*	21.43461	1.40852
96IleCb	96IleHb	41.76466	1.76069
96IleCd1	96IleHd1*	15.15905	0.85493
96IleCg1	96IleHg1a	27.85134	1.7839
96IleCg2	96IleHg2*	17.71295	0.94337
101ThrCa	101ThrHa	62.59618	4.42385
101ThrCb	101ThrHb	69.27951	4.2223
101ThrCg2	101ThrHg2*	20.67039	1.14961
103AlaCa	103AlaHa	54.23794	4.16106
103AlaCb	103AlaHb*	17.67285	1.60693
104PheCa	104PheHa	59.00477	4.45473
104PheCb	104PheHba	37.66073	2.91955
105MetCa	105MetHa	59.30037	3.9678
105MetCb	105MetHbb	31.78518	1.9352
105MetCb	105MetHba	31.77292	1.79661
105MetCg	105MetHg*	28.66897	2.0861
106GluCa	106GluHa	58.6629	3.92197
106GluCb	106GluHb*	28.69815	2.09817
106GluCg	106GluHgb	36.10107	2.42457
106GluCg	106GluHga	36.07637	2.20313
107AlaCa	107AlaHa	54.35369	4.12627
107AlaCb	107AlaHb*	16.56033	1.33944
108LeuCa	108LeuHa	56.86384	4.15069
108LeuCb	108LeuHba	40.76246	1.49395
108LeuCb	108LeuHbb	40.76115	1.84598
108LeuCda	108LeuHda*	21.38347	0.86736
108LeuCdb	108LeuHdb*	24.25606	0.9617
109SerCa	109SerHa	60.62758	4.22131
109SerCb	109SerHb*	62.29115	3.97042
110AlaCa	110AlaHa	51.38212	4.49703
110AlaCb	110AlaHb*	18.44893	1.48718
111GlyCa	111GlyHab	44.89535	4.34909
111GlyCa	111GlyHaa	44.89535	3.78726

112AlaCa	112AlaHa	51.83506	4.36342
112AlaCb	112AlaHb*	18.8786	1.26998
113AspCa	113AspHa	53.89673	4.42583
113AspCb	113AspHba	41.82812	2.67126
113AspCb	113AspHbb	41.83417	2.8177
114?ValCG2|CG1[3059]	None	26.60563	-0.03521
114?ValCG2|CG1[3060]	None	23.22509	-0.49862
115SerCa	115SerHa	60.52828	4.26503
115SerCb	115SerHba	62.58412	4.18148
115SerCb	115SerHbb	62.61035	4.34476
116MetCa	116MetHa	56.29649	4.51168
116MetCb	116MetHb*	31.90453	2.50848
116MetCg	116MetHga	30.68081	2.63724
116MetCg	116MetHgb	30.68081	2.65442
117IleCd1	117IleHd1*	14.93555	0.7778
117IleCg2	117IleHg2*	19.73822	0.94015
118GlyCa	118GlyHab	45.48629	3.74976
118GlyCa	118GlyHaa	45.48253	3.72342
119GlnCa	119GlnHa	56.17739	4.21154
119GlnCb	119GlnHb*	27.9243	1.88852
119GlnCg	119GlnHgb	33.32828	2.23588
119GlnCg	119GlnHga	33.33015	2.22472
122ValCa	122ValHa	59.8004	4.67363
122ValCb	122ValHb	32.05848	2.78359
122ValCga	122ValHga*	17.66504	0.57077
122ValCgb	122ValHgb*	22.13166	0.90468
125TyrCa	125TyrHa	60.85456	4.30145
125TyrCb	125TyrHba	37.07664	3.1206
125TyrCb	125TyrHbb	37.11243	3.1874
126SerCa	126SerHa	61.46945	3.8582
126SerCb	126SerHbb	64.23782	3.85539

126SerCb	126SerHba	64.17353	3.77945
127LeuCa	127LeuHa	58.04818	3.80412
127LeuCb	127LeuHb*	40.32938	1.18745
127LeuCda	127LeuHda*	23.07523	0.51765
127LeuCdb	127LeuHdb*	23.06647	0.51239
127LeuCg	127LeuHg	26.50409	1.29225
128PheCa	128PheHa	60.19967	4.92482
128PheCb	128PheHbb	37.03838	3.47944
128PheCb	128PheHba	37.05447	2.6635
129LeuCa	129LeuHa	56.91583	4.26494
129LeuCb	129LeuHb*	42.26855	1.71335
129LeuCda	129LeuHda*	23.18569	0.57349
129LeuCdb	129LeuHdb*	24.68686	0.85751
129LeuCg	129LeuHg	26.47786	1.2764
130ValCa	130ValHa	59.78581	4.56082
130ValCb	130ValHb	32.37998	2.0001
130ValCga	130ValHga*	14.82513	-0.60784
130ValCgb	130ValHgb*	21.59859	0.45012
131AlaCa	131AlaHa	50.2802	5.0646
131AlaCb	131AlaHb*	21.54701	1.05055
133ArgCa	133ArgHa	54.40983	5.09444
133ArgCb	133ArgHb*	33.24854	1.9282
133ArgCd	133ArgHdb	42.78086	2.73412
133ArgCd	133ArgHda	42.76442	2.46331
133ArgCg	133ArgHgb	26.54901	1.70085
133ArgCg	133ArgHga	26.55988	1.51485
134ValCa	134ValHa	58.28415	5.69762
134ValCb	134ValHb	34.72703	1.92653
134ValCga	134ValHga*	22.12681	0.91141
134ValCgb	134ValHgb*	20.56829	1.26678
136ValCa	136ValHa	60.99422	4.89837
136ValCb	136ValHb	33.10556	2.28511
136ValCga	136ValHga*	21.05395	0.4209

137IleCa	137IleHa	59.53411	4.48899
137IleCb	137IleHb	38.99022	1.92093
137IleCd1	137IleHd1*	14.64787	0.82885
137IleCg1	137IleHg1a	28.2394	1.09014
137IleCg1	137IleHg1b	28.23283	1.5469
137IleCg2	137IleHg2*	19.08631	0.97873
138SerCa	138SerHa	56.70057	5.53419
138SerCb	138SerHba	66.31571	3.6235
138SerCb	138SerHbb	66.34168	3.86151
140SerCa	140SerHa	54.52089	4.95332
140SerCb	140SerHba	63.27118	3.37313
140SerCb	140SerHbb	63.28265	3.60094
141AsnCa	141AsnHa	54.76372	4.42184
141AsnCb	141AsnHb*	36.6846	2.8387
142AspCa	142AspHa	54.00444	4.72775
142AspCb	142AspHba	41.31462	2.76412
142AspCb	142AspHbb	41.31462	2.94875
143AspCa	143AspHa	52.73346	5.06653
144GluCa	144GluHa	53.8629	4.47669
144GluCb	144GluHb*	30.55401	2.35881
144GluCg	144GluHg*	36.02025	2.3732
145GlnCa	145GlnHa	55.99578	5.1485
145GlnCb	145GlnHb*	29.08252	2.01293
145GlnCg	145GlnHgb	34.08945	2.42694
145GlnCg	145GlnHga	34.08945	2.28161
146TyrCa	146TyrHa	58.30921	5.02892
147IleCa	147IleHa	59.80933	5.10823
147IleCb	147IleHb	41.32915	1.81124
147IleCd1	147IleHd1*	13.73075	0.79506
147IleCg1	147IleHg1*	28.97046	1.76153
147IleCg2	147IleHg2*	17.77735	0.93489
148TrpCa	148TrpHa	55.40834	5.97427
148TrpCb	148TrpHba	34.35812	2.93167

149GluCa	149GluHa	54.72573	5.73187
149GluCb	149GluHb*	32.49982	2.1229
149GluCg	149GluHg*	36.31851	2.14402
150SerCa	150SerHa	57.3507	4.85933
150SerCb	150SerHba	67.29989	3.75501
150SerCb	150SerHbb	67.29989	3.82543
151AsnCa	151AsnHa	51.88486	5.35147
151AsnCb	151AsnHbb	38.23703	2.82411
151AsnCb	151AsnHba	38.2326	2.79314
152AlaCb	152AlaHb*	16.36045	1.19427
153GlyCa	153GlyHaa	44.85505	3.86516
153GlyCa	153GlyHab	44.8649	4.30452
154GlyCa	154GlyHaa	45.68805	3.80943
154GlyCa	154GlyHab	45.75833	4.21105
155SerCa	155SerHa	56.14159	5.3335
155SerCb	155SerHbb	66.2724	3.69165
155SerCb	155SerHba	66.26734	3.63646
156PheCa	156PheHa	54.63854	5.21741
157ThrCa	157ThrHa	58.51398	5.63745
157ThrCb	157ThrHb	72.05808	3.96593
157ThrCg2	157ThrHg2*	20.83556	1.10765
158ValCa	158ValHa	61.15287	5.57437
158ValCb	158ValHb	34.90492	2.10377
158ValCga	158ValHga*	22.18312	1.06956
158ValCgb	158ValHgb*	22.64972	1.28314
159ThrCa	159ThrHa	61.00846	5.07005
159ThrCb	159ThrHb	71.73493	3.85428
159ThrCg2	159ThrHg2*	20.37815	1.38555
160LeuCa	160LeuHa	56.29956	3.68907
160LeuCb	160LeuHbb	40.85137	1.31529
160LeuCb	160LeuHba	40.90778	1.27235
160LeuCda	160LeuHda*	22.87462	0.56856
160LeuCdb	160LeuHdb*	24.78293	0.93038

160LeuCg	160LeuHg	27.1767	1.27771
161AspCa	161AspHa	53.87606	4.45817
161AspCb	161AspHb*	41.82408	2.76975
162GluCa	162GluHa	54.70196	4.73903
162GluCb	162GluHb*	30.05262	2.34126
162GluCg	162GluHg*	36.48239	2.07717
163ValCa	163ValHa	62.04897	4.49895
163ValCb	163ValHb	34.64423	1.99514
163ValCga	163ValHga*	20.63891	0.85937
163ValCgb	163ValHgb*	18.76776	0.86259
164AsnCa	164AsnHa	53.56482	4.83988
164AsnCb	164AsnHb*	38.8113	2.60472
165GluCa	165GluHa	56.16205	4.13502
165GluCb	165GluHba	28.74953	1.95888
165GluCb	165GluHbb	28.74539	1.98743
165GluCg	165GluHg*	35.35846	2.16634
166ArgCa	166ArgHa	54.30589	4.41544
166ArgCb	166ArgHb*	30.34261	1.82114
166ArgCd	166ArgHda	42.79565	3.16566
166ArgCd	166ArgHdb	42.80335	3.23264
166ArgCg	166ArgHg*	27.04671	1.69968
167IleCa	167IleHa	59.98275	4.15481
167IleCb	167IleHb	39.32263	1.61164
167IleCd1	167IleHd1*	13.6784	0.57033
167IleCg1	167IleHg1*	25.94714	1.27831
167IleCg2	167IleHg2*	17.67812	0.6871
169ArgCa	169ArgHa	55.87942	4.44363
169ArgCb	169ArgHb*	30.33579	1.89451
169ArgCd	169ArgHd*	42.7232	3.18573
169ArgCg	169ArgHg*	26.59071	1.67061
170GlyCa	170GlyHab	43.00396	3.82994
170GlyCa	170GlyHaa	43.02548	3.85791
171ThrCa	171ThrHa	61.8091	5.37648

171ThrCb	171ThrHb	71.39526	4.21085
171ThrCg2	171ThrHg2*	22.27519	0.76424
172IleCa	172IleHa	61.17033	4.73149
172IleCb	172IleHb	40.06981	1.8522
172IleCd1	172IleHd1*	15.49372	0.85856
172IleCg1	172IleHg1a	28.17121	1.07646
172IleCg1	172IleHg1b	28.16348	1.53387
172IleCg2	172IleHg2*	16.89231	0.77372
173LeuCa	173LeuHa	53.1948	4.92799
173LeuCb	173LeuHb*	41.97842	1.55939
173LeuCda	173LeuHda*	25.70252	1.00305
173LeuCg	173LeuHg	29.1217	1.90782
174ArgCa	174ArgHa	55.80816	4.43898
174ArgCb	174ArgHb*	30.81775	1.85654
174ArgCd	174ArgHdb	42.20087	3.26142
174ArgCd	174ArgHda	42.18799	3.12881
174ArgCg	174ArgHg*	26.80999	1.62927
175LeuCa	175LeuHa	54.27214	4.48573
175LeuCb	175LeuHb*	42.00033	1.73602
175LeuCda	175LeuHda*	26.12443	0.64697
175LeuCdb	175LeuHdb*	25.38797	0.78203
175LeuCg	175LeuHg	27.99867	1.56997
176PheCa	176PheHa	56.77167	4.62804
177LeuCa	177LeuHa	55.82335	4.37168
177LeuCb	177LeuHba	41.85194	1.59461
177LeuCda	177LeuHda*	21.86848	0.63731
177LeuCdb	177LeuHdb*	26.50467	0.83898
178LysCa	178LysHa	55.87504	4.28716
178LysCe	178LysHeb	41.42464	3.00519
178LysCe	178LysHea	41.42731	2.89135
179AspCa	179AspHa	56.7272	4.36237
179AspCb	179AspHb*	40.19448	2.70137
180AspCa	180AspHa	52.70013	4.86233

180AspCb	180AspHbb	39.12352	3.09435
180AspCb	180AspHba	39.11641	2.66226
181GlnCa	181GlnHa	53.3936	4.9828
181GlnCb	181GlnHba	26.66035	1.95791
181GlnCb	181GlnHbb	26.65485	1.97387
181GlnCg	181GlnHg*	32.16628	2.39806
182LeuCa	182LeuHa	55.8732	4.08055
182LeuCb	182LeuHb*	38.17224	1.88796
182LeuCda	182LeuHda*	22.04939	0.7516
182LeuCdb	182LeuHdb*	25.21641	1.03078
182LeuCg	182LeuHg	29.10327	1.94495
183GluCa	183GluHa	57.68444	4.181
183GluCb	183GluHb*	27.89567	2.09151
183GluCg	183GluHga	35.64601	2.29447
183GluCg	183GluHgb	35.63107	2.44149
184TyrCa	184TyrHa	59.71588	4.23372
184TyrCb	184TyrHb*	37.03928	2.69396
185LeuCa	185LeuHa	53.54604	4.40929
185LeuCda	185LeuHda*	24.25751	0.65851
185LeuCdb	185LeuHdb*	25.32257	0.76872
185LeuCg	185LeuHg	27.76593	1.01985
186GluCa	186GluHa	54.74525	4.34475
186GluCb	186GluHb*	29.11034	2.23047
186GluCg	186GluHga	35.6321	2.25337
186GluCg	186GluHgb	35.61044	2.41493
187GluCa	187GluHa	59.77642	4.71204
187GluCb	187GluHb*	28.73648	2.05686
187GluCg	187GluHgb	37.45103	2.39635
187GluCg	187GluHga	37.4468	2.34084
188LysCa	188LysHa	59.38346	3.94051
188LysCb	188LysHba	31.75125	1.78208
188LysCb	188LysHbb	31.75125	1.91882
188LysCd	188LysHdb	28.90995	1.70478

188LysCd	188LysHda	28.90398	1.66796
188LysCe	188LysHe*	41.40337	2.98819
188LysCg	188LysHgb	24.39897	1.52073
188LysCg	188LysHga	24.38669	1.42067
189ArgCa	189ArgHa	56.48194	4.19707
189ArgCb	189ArgHb*	29.08224	1.99594
189ArgCd	189ArgHd*	41.31108	3.22316
189ArgCg	189ArgHg*	24.42188	1.51014
190IleCa	190IleHa	65.30699	3.47638
190IleCb	190IleHb	37.64378	1.9105
190IleCd1	190IleHd1*	13.1276	0.89768
190IleCg1	190IleHg1b	29.03932	1.78254
190IleCg1	190IleHg1a	29.03932	1.05156
190IleCg2	190IleHg2*	18.55192	0.93731
191LysCa	191LysHa	60.22202	3.81252
191LysCb	191LysHba	31.7396	1.86236
191LysCb	191LysHbb	31.74123	1.87931
191LysCd	191LysHdb	29.07457	1.93344
191LysCd	191LysHda	29.04081	1.66772
191LysCe	191LysHe*	41.47305	2.9484
191LysCg	191LysHg*	26.57018	1.68964
192GluCa	192GluHa	58.65188	4.05669
192GluCb	192GluHbb	29.10002	2.30399
192GluCb	192GluHba	29.08194	1.52891
192GluCg	192GluHgb	36.06788	2.45107
192GluCg	192GluHga	36.06622	2.21114
193ValCa	193ValHa	66.81092	3.7794
193ValCb	193ValHb	31.24692	2.28487
193ValCga	193ValHga*	23.48518	1.01409
193ValCgb	193ValHgb*	23.66969	1.30129
194IleCa	194IleHa	64.75796	3.59684
194IleCb	194IleHb	37.41135	1.82311
194IleCd1	194IleHd1*	13.72795	0.78506

194IleCg1	194IleHg1a	28.8508	1.18243
194IleCg2	194IleHg2*	16.96977	0.80445
195LysCa	195LysHa	58.00386	3.96132
195LysCb	195LysHba	30.84156	1.85125
195LysCb	195LysHbb	30.83436	2.01108
195LysCd	195LysHd*	28.23848	1.70562
195LysCe	195LysHe*	41.55608	2.95624
195LysCg	195LysHg*	24.34832	1.42996
196ArgCa	196ArgHa	57.97515	3.98232
196ArgCb	196ArgHbb	30.54013	1.48013
196ArgCb	196ArgHba	30.54469	1.46027
196ArgCd	196ArgHda	42.87922	3.09799
196ArgCd	196ArgHdb	42.88207	3.12481
196ArgCg	196ArgHg*	26.65188	1.48537
197HisCa	197HisHa	56.79846	4.90274
197HisCb	197HisHb*	33.59027	2.808
198SerCa	198SerHa	57.28966	4.77517
198SerCb	198SerHba	63.32373	3.688
198SerCb	198SerHbb	63.30761	4.09304
199GluCa	199GluHa	58.04912	3.8201
199GluCb	199GluHbb	29.03077	1.71334
199GluCb	199GluHba	29.03785	1.56471
199GluCg	199GluHga	35.48851	1.65509
199GluCg	199GluHgb	35.47766	1.86812
200PheCa	200PheHa	56.30114	4.66886
200PheCb	200PheHba	37.68939	2.94065
200PheCb	200PheHbb	37.66242	3.28376
201ValCa	201ValHa	62.30466	3.98024
201ValCb	201ValHb	31.88929	2.06917
201ValCga	201ValHga*	21.87254	0.95018
201ValCgb	201ValHgb*	20.52762	1.09921
202AlaCa	202AlaHa	52.30923	4.13101
202AlaCb	202AlaHb*	18.45713	1.08985

203TyrCa	203TyrHa	55.13992	4.72458
203TyrCb	203TyrHb*	39.79735	2.96432
205IleCa	205IleHa	59.79245	4.69027
205IleCb	205IleHb	37.8658	1.74487
205IleCd1	205IleHd1*	13.64648	0.89213
205IleCg1	205IleHg1*	27.19322	1.59505
205IleCg2	205IleHg2*	16.71952	0.71201
206GlnCb	206GlnHba	28.72565	2.06707
206GlnCb	206GlnHbb	28.72565	2.10078
206GlnCg	206GlnHga	35.6751	2.30463
206GlnCg	206GlnHgb	35.68546	2.51234
207LeuCa	207LeuHa	56.41434	4.73403
207LeuCb	207LeuHbb	44.39191	1.72646
207LeuCb	207LeuHba	44.40276	1.52736
207LeuCda	207LeuHda*	25.94565	0.90639
207LeuCdb	207LeuHdb*	24.76988	0.91278
207LeuCg	207LeuHg	27.71533	1.70428