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Biochemistry, 1996, 35(2), 418-426, DOI:[10.1021/bi9520287](https://doi.org/10.1021/bi9520287)

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Table S1

Proton Assignments for LSIII, pH 4.6 and 25° C (in ppm).

Residue	H ^N	H ^α	H ^β	Others
Arg 1	8.396	5.249	1.675	H ^γ 1.805, H ^δ 2.004
Glu 2	8.327	5.063	2.479	H ^γ 3.068
Cys 3	9.538	4.431	2.528, 3.026	
Tyr 4	8.496	3.933	3.268, 3.092	H ^δ 6.871, H ^ε 6.651
Leu 5	9.477	3.260	1.950	H ^γ 0.541 H ^δ 1.515, 0.991
Asn 6	8.913	4.977	2.594	H ^ε 6.463
Pro 7		4.331	2.077, 1.768	H ^γ 2.262, 1.253 H ^δ 3.569, 3.447
His 8	7.447	4.554		H ^δ 8.543
Asp 9	7.354	3.643	1.412	
Thr 10	8.335	4.965	3.691	H ^γ 0.141
Gln 11	8.606	4.627	1.892	H ^γ 2.133, 2.266
Thr 12	8.609	4.497	3.928	H ^γ 1.246
Cys 13	9.143	4.870	2.806, 3.304	
Pro 14		4.429	2.131, 1.654	H ^γ 2.000, 1.958 H ^δ 3.887 3.418
Ser 15	7.880	4.664	3.972, 3.893	
Gly 16	8.946	4.299, 3.758		
Gln 17	9.059	5.023	2.376	H ^γ 2.876
Glu 18	8.412	4.539	1.828	H ^γ 3.059, 2.964
Ile 19	8.509	4.627	1.892	H ^γ 0.906 , 1.207 H ^δ 0.699
Cys 20	9.069	5.957	3.146	
Tyr 21	9.086	6.424	3.032, 2.636	H ^δ 6.884, H ^ε 6.729
Val 22	8.894	5.127	1.839	H ^γ 0.779, -0.025
Lys 23	9.818	5.493	1.929, 1.352	H ^γ 1.574, 1.330 H ^δ 2.469
Ser 24	9.225	5.679	3.318, 3.033	

K-426-DN2

Trp 25	8.686	5.155	3.181, 3.745	H ^δ 7.177, H ^{ε3} 7.556 H ^{ε3} 7.140, H ^η 7.226 H ^{ε2} 7.482, H ^{ε1} 10.091
Cys 26	9.049	5.077	2.985, 3.325	
Asn 27	8.355	4.911	3.308, 2.853	H ^δ 7.809
Ala 28	8.193	4.000	0.921	
Trp 29	7.925	4.873	3.487, 3.171	H ^δ 6.896, H ^{ε3} 6.719 H ^{ε3} 7.128, H ^η 7.130 H ^{ε2} 7.409, H ^{ε1} 10.201
Cys 30	7.849	4.166	3.495, 3.177	
Ser 31	8.376	4.096	3.793	
Ser 32	7.962	4.339	3.716	
Arg 33	8.250	4.397	1.835	H ^γ 2.371
Gly 34	7.712	4.271, 3.921		
Lys 35	8.071	4.144	1.345	H ^γ 1.475
Val 36	8.534	3.516	0.258	H ^γ 0.495, 0.403
Leu 37	7.434	5.073	1.498, 1.162	H ^γ 0.662 H ^δ 0.570, -0.308
Glu 38	9.035	5.415	2.852, 2.705	H ^γ 3.698
Phe 39	9.477	5.043	3.444	H ^δ 7.012, H ^ε 7.165 H ^ε 7.242
Gly 40	7.016	4.097, 3.799		
Cys 41	8.286	5.689	3.450, 3.026	
Ala 42	9.583	4.535	1.503	
Ala 43	8.952	4.772	1.535	
Thr 44	7.360	4.333	3.981	H ^γ 1.086
Cys 45	8.925	4.579	2.855, 3.092	
Pro 46		4.089	2.006, 1.253	H ^γ 0.538 H ^δ 3.069, 3.729
Ser 47	7.847	4.337	2.092, 2.263	H ^γ 0.668
Val 48	8.253	4.520	2.057	
Asn 49	8.221	4.795	2.631, 2.809	
Thr 50	8.863	4.292	4.022	H ^γ 1.258
Gly 51	8.971	4.386, 3.793		
Thr 52	8.140	5.016	4.153	H ^γ 1.188
Glu 53	8.977	4.726	2.078	H ^γ 2.293
Ile 54	8.866	5.306	1.553	H ^γ 0.860

K-426-m3

Lys 55	8.363	4.729	1.833, 1.740	H ^γ 1.545, 0.903 H ^δ 2.961 H ^ε 7.563
Cys 56	8.318	4.849	3.191, 3.083	
Cys 57	8.557	4.707	2.183, 2.314	
Ser 58	9.041	5.173	3.890	
Ala 59	7.279	4.556	1.387	
Asp 60	8.396	4.980	2.755, 2.438	
Lys 61	8.689	4.464	1.514, 1.638	H ^γ 0.869, 0.774
Cys 62	7.631	4.729	3.599, 3.263	
Asn 63	9.373	4.537	2.649, 2.279	
Thr 64	7.350	4.006	3.981	
Tyr 65	8.634	4.657	2.863, 2.645	
Pro 66		4.882	3.196, 3.355	H ^γ 1.599, 1.505 H ^δ 3.080, 3.115