

SUPPORTING INFORMATION FOR WORLD WIDE WEB EDITION

Table 1 Proton resonance assignments (ppm) for MSTI at 27 °C and pH 5.6

Residue	HN	H α	H β	H γ	H δ	Others
THR 1	-	4.15	3.88	1.32		
LYS 2						
SER 3	8.58	4.56	3.92 3.88			
THR 4	8.38	4.46	4.32	1.24		
THR 5	8.23	4.50	4.30	1.21		
THR 6	8.07	4.29	4.24	1.21		
ALA 7	8.04	4.01	0.50			
CYS 8	7.23	5.12	2.98 2.93			
CYS 9	9.20	4.67	3.09 2.86			
ASP 10	11.52	4.93	2.60 2.21			
PHE 11	9.31	4.67	3.07 3.00			H _{2,6} 7.37 H _{3,5} 7.3
CYS 12	8.56	6.01	3.44 3.11			
PRO 13		4.59	2.16	1.93	3.22	
CYS 14	8.27	5.72	2.97 2.86			
THR 15	8.78	4.42	4.56	1.40		
ARG 16	8.61	4.51	2.09 2.07	1.73 1.70	3.23	
SER 17	7.30	4.39	3.89 3.76			
ILE 18	8.26	4.28	1.79	1.06 1.46 1.19	0.86	
PRO 19		5.12	2.60 2.08	2.00 1.92	3.59	
PRO 20		4.17	2.37 2.09	1.88	3.81 3.79	
GLN 21	7.50	4.59	2.26 2.16	1.80		H ϵ 7.52 6.82
CYS 22	9.55	5.55	2.60 2.44			
GLN 23	7.74	4.77	2.34 2.13	2.00 1.80		H ϵ 7.24 6.84
CYS 24	9.28	5.44	3.24 3.18			
THR 25	9.18	4.34	4.48	1.05		
ASP 26	7.66	4.42	2.77 2.63			
VAL 27	8.61	4.82	1.96	0.99 0.86		
ARG 28	8.50	4.95	2.17 2.00	1.71 1.62	3.36 3.32	NH 7.28 7.34
GLU 29	9.09	4.42	2.10 2.00	2.37 2.30		
LYS 30	7.28	4.57	1.90 1.75	1.30 1.17	1.66	H ϵ 2.98
CYS 31	8.69	4.64	3.34 2.84			
HIS 32	8.29	4.57	3.43 3.30			H ₂ 7.19 H ₄ 7.45
SER 33	8.49	4.12	4.01 3.91			
ALA 34	9.00	4.68	1.14			
CYS 35	7.29	4.37	3.04			
LYS 36	11.54	4.40	2.07 1.92	1.63 1.50	1.74	H ϵ 3.07
SER 37	9.39	4.62	3.91 3.71			
CYS 38	8.69	5.33	3.13 2.68			
LEU 39	8.91	4.92	1.78 1.72	1.53	0.78 0.66	
CYS 40	8.97	5.87	3.08 2.90			
THR 41	8.70	4.41	4.52	1.39		
ARG 42	8.60	4.45	2.08 2.04	1.71 1.63	3.23	
SER 43	7.30	4.38	3.88 3.76			
PHE 44	8.47	4.69	3.04 2.94			H _{2,6} 7.29 H _{3,5} 7.3

PRO 45		4.38	2.18 1.86	1.76	3.49 3.41	
PRO 46		4.16	2.36 2.27	2.12 2.01	3.71 3.59	
GLN 47	7.47	4.37	2.19 2.10	1.72		H ϵ 6.81 7.45
CYS 48	9.59	5.53	2.94 2.52			
ARG 49	8.59	4.70	1.72 1.39	1.14	2.86 2.63	NH ₂ 6.83 7.25
CYS 50	9.86	5.24	3.19 2.84			
TYR 51	9.70	4.50	3.43 2.70			H _{2,6} 6.83 H _{3,5} 7.2
ASP 52	7.50	4.42	2.73			
ILE 53	8.60	5.01	1.86	0.95 1.63 1.27	0.83	
THR 54	8.98	4.78	3.79	0.98		
ASP 55	8.39	4.97	3.036 2.62			
PHE 56	6.84	4.70	3.00 2.87			H _{2,6} 6.97 H _{3,5} 6.6 H ₄ 7.06
CYS 57	8.65	4.73	3.08 3.72			
TYR 58	8.74	4.44	3.01 2.16			H _{2,6} 6.73 H _{3,5} 6.9
PRO 59		4.56	2.42 2.10	2.00	3.94	
SER 60	8.29	4.68	4.06 4.02			
CYS 61	8.19	4.56	3.28 3.21			
SER 62	8.47	4.28	3.84 3.80			