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Table I: Chemical Shifts for the Assigned Proton NMR Resonances of Iron (II) c552 from H. thermophilus at 25 °C and pH 4.8

residue	NH	CαH	CβH	Others
N1	n.a.	2.90	2.25*	NH2 n.a.
E2	7.95	2.94	1.95, 1.87	CγH2 2.39
Q3	7.90	3.98	2.07	CγH2 2.43 NH2 n.a.
L4	7.81	4.24	1.74	CγH 1.61 CδH3 1.10, 1.00
A5	7.81	4.33	1.40	
K6	8.16	4.22	2.02, 1.70	CγH2 1.47 CδH2 1.75 CεH2 3.04
Q7	8.53	4.21	2.47, 2.37	CγH2 2.71, 2.58 NH2 n.a.
K8	8.45	4.75	2.74, 2.03	CγH2 1.45 CδH2 2.04 CεH2 3.07
G9	7.95	4.86, 4.32		
C10	8.96	5.13	3.26, 2.63	
M11	7.97	4.70	2.76	CγH2 2.13, 2.37 CεH3 1.99
A12	7.69	4.27	1.78	
C13	6.58	4.31	1.84, 0.96	
H14	6.77	3.39	0.86, -0.09	Nδ1H 9.01 Cε1H 0.70 Cδ2H 0.84
D15	7.62	4.46	2.79, 2.04	
L16	8.30	3.77	1.80, 1.52	CγH 1.80 CδH3 1.12, 1.02
K17	8.03	4.40	1.82, 1.58	CγH2 1.21 CδH2 1.59 CεH2 2.89
A18	8.15	4.43	1.18	
K19	8.37	3.64	1.71	CγH2 1.16 CδH2 1.59 CεH2 2.92
K20	7.47	4.29	1.30	CγH2 1.01 CδH2 1.19 CεH2 2.61
V21	7.15	4.06	1.87	CγH3 1.64, 1.19
G22	6.62	3.78, 0.18		
P23	----	3.60	0.89, 0.45	CγH2 0.21, 0.12 CδH2 2.95, 2.19
A24	8.36	3.86	0.70	
Y25	7.83	4.06	2.72,2.39	CδH 6.00 CεH 4.92[a]
A26	8.81	4.01	1.38	
D27	6.83	4.06	2.83, 2.72	
V28	7.67	4.15	2.40	CγH3 1.77, 0.86
A29	8.45	4.07	1.77	
K30	7.41	4.19	2.04, 1.78	CγH2 1.60 CδH2 1.83 CεH2 3.09
K31	7.99	4.04	2.04, 1.87	CγH2 0.46 CδH2 1.33 CεH2 n.a.
Y32	7.54	4.28	3.61, 2.75	CδH 7.53 CεH 7.30
A33	7.52	4.27	1.64	
G34	8.81	4.09, 4.05		
R35	7.92	4.66	2.30, 2.16	CγH2 1.94, 1.84 CδH2 3.46, 3.09
				εNH 8.26 ηNH2 6.60
K36	9.23	4.27	2.02, 2.00	CδH2 1.65 CδH2 1.84 CεH2 3.15
D37	8.83	5.03	3.17, 2.75	
A38	7.50	3.99	1.86	
V39	7.73	3.55	2.16	CγH3 1.12, 1.09
D40	7.73	4.38	2.71, 2.71	

residue	HN	Hα	Hβ	Others
Y41	8.51	4.16	3.27, 2.78	Cδ1H 6.80 Cε1H 6.76
L42	8.86	3.65	2.22, 1.38	CγH 2.04 Cδ1H3 1.17, 1.09
A43	8.79	3.92	1.44	
G44	7.40	3.80, 3.70		
K45	7.20	3.52	1.42, 1.33	Cγ2H2 1.11 Cδ2H2 1.31 Cε2H2 n.a.
I46	8.02	1.84	1.56	Cγ2H2 1.22, 1.35 Cγ1H3 0.69 Cδ1H3 1.21
K47	6.83	3.80	1.76, 1.53	Cγ2H2 1.32 Cδ2H2 1.64 Cε2H2 2.98
K48	7.89	3.95	1.64, 1.53	Cγ2H2 1.33 Cδ2H2 1.41 Cε2H2 n.a.
G49	7.08	3.10, 1.87		
G50	7.50	4.32, 3.64		
S51	8.09	4.51	3.93, 3.65	
G52	8.07	4.67, 4.04		
V53	10.38	4.00	2.69	Cγ1H3 1.21, 0.78
W54	10.56	4.81	3.93, 3.67	Cδ1H 7.86 Cε3H 8.09 Cζ3H 7.34 Cζ2H 7.11 Cη2H 7.64 Nε1H 12.34
G55	8.12	4.61, 4.25		
S56	8.87	4.83	4.17, 4.04	
V57	7.81	4.66	2.37	Cγ1H3 1.41, 1.36
P58	----	4.67	2.20, 1.59	Cγ2H2 2.20 Cδ2H2 4.22, 3.97
M59	8.56	3.67	-0.55, -2.52	Cγ2H2 -0.99, -3.56 Cε1H3 -2.82
P60	----	4.40	1.94, 1.52	Cγ2H2 2.32 Cδ2H2 3.93, 2.68
P61	----	3.39	2.08, 1.66	Cγ2H2 2.57, 1.83 Cδ2H2 3.45, 3.38
Q62	7.31	4.32	1.94, 1.71	Cγ2H2 1.44, 1.21 Nε2H2 6.64, 6.41
N63	8.98	4.89	3.05, 2.76	Nδ2H2 7.69, 6.93
V64	7.50	4.97	2.53	Cγ1H3 0.90, 0.71
T65	9.17	4.54	4.84	Cγ2H3 1.38
D66	8.93	4.33	2.72, 2.72	
A67	8.41	4.19	1.50	
E68	7.99	4.02	2.37, 1.78	Cγ2H2 2.63, 2.56
A69	8.92	4.07	1.67	
K70	8.01	3.99	1.96	Cγ2H2 1.34 Cδ2H2 1.71 Cε2H2 2.90
Q71	8.13	4.23	2.35, 2.20	Cγ2H2 2.63, 2.44 Nε2H2 6.84, (6.83)
L72	9.00	4.42	2.51, 1.79	Cγ1H 2.11 Cδ1H3 1.31, 1.22
A73	8.63	4.10	1.78	
Q74	8.50	4.00	2.39, 2.23	Cγ2H2 2.52, 2.72 Nε2H2 7.37
W75	8.17	4.49	3.68, 3.49	Cδ1H 7.38 Cε3H 7.60 Cζ3H 6.54 Cζ2H 6.87 Cη2H 7.35 Nε1H 10.43
I76	8.81	2.55	1.83	Cγ2H2 1.69, -0.63 Cγ1H3 0.70 Cδ1H3 1.08
L77	7.74	3.96	1.99, 1.90	Cγ1H 1.73 Cδ1H3 1.10, 0.97
S78	7.83	4.52	4.21, 4.05	
I79	7.27	3.72	1.72	Cγ2H2 1.00, 0.91 Cγ1H3 0.71 Cδ1H3 0.04
K80	7.74	4.26	1.89	Cγ2H2 1.43 Cδ2H2 n.a. Cε2H2 3.08

heme assignments[b]								
α meso	9.86	4-H	6.27	5-methyl	3.39	6-porp(6L1)	4.66,	4.37
β meso	9.43	2-H	6.21	8-methyl	3.51	6-porp(6L2)	3.54,	2.77
γ meso	9.49	3-methyl	3.93	4-methyl	2.49	7-prop(7L1)	4.66,	4.20
δ meso	9.34	1-methyl	3.75	2-methyl	2.06	7-prop(7L2)	3.64,	2.89

All chemical shift values are given in ppm with respect to H_2O, which in turn was calibrated by using internal 2,2-dimethyl-2-silapentane-5-sulfonate(DSS). a Tyr 25 (3,5) protons chemical shift at 60 °C. b IUPAC/IUB nomenclature used for heme propionates indicatd parenthetically. * tentative assignment. n.a., not assigned