Table 1 ^{15}N, ^{13}C, ^{13}CO and ^{1}H resonance assignments for collagenase at pH 6.5 and 25°C.[a]

Residue	N	CO	Cα	Cβ	Others
V1	- (-)	172.0	60.8 (3.86)	32.5 (2.25)	Cγ 19.4(1.06);Cγ 20.1(1.06)
L2	- (-)	176.7	55.0 (4.53)	41.9 (1.68)	Cγ 26.9(1.68);Cδ 24.2(0.98);Cδ 23.6(0.93)
T3	114.3 (8.28)	173.9	61.5 (4.34)	69.4 (4.21)	Cγ 21.3(1.22)
E4	121.6 (8.43)	176.3	56.5 (4.31)	30.1 (2.08,1.99)	Cγ 35.9(2.28)
G5	107.9 (8.43)	173.2	44.7 (4.00,3.93)		
N6	117.7 (8.27)	172.8	51.4 (4.92)	38.4 (2.87,2.63)	
P7	- (-)	174.5	62.9 (4.40)	32.2 (2.20,1.76)	Cγ 27.3(1.98);Cδ 50.1(3.68)
R8	111.8 (7.82)	174.9	53.8 (4.58)	32.6 (1.76,1.64)	Cγ 24.3(1.65,1.20);Cδ 43.3(3.14,2.92)
W9	120.1 (8.09)	176.9	56.9 (4.71)	29.9 (3.65,3.24)	Cδ1 126.7(7.43);Nε1 125.7(10.47); Cζ2 112.9(7.51);Cε3 - (7.92)
E10	121.8 (9.27)	176.1	57.2 (4.40)	29.7 (2.31,2.11)	Cγ 36.1(2.44,2.37);Nε2 110.5(6.90,7.56)
Q11	116.0 (8.43)	174.1	54.0 (4.71)	29.8 (2.22)	Cγ 32.9(2.42)
T12	103.7 (7.97)	172.6	61.1 (4.29)	68.9 (4.32)	Cγ 21.4(1.20)
H13	117.4 (7.31)	173.3	53.4 (5.11)	28.7 (3.02,2.97)	Cδ -(7.01)
L14	124.8 (8.23)	176.3	53.1 (4.59)	45.5 (1.46,1.05)	Cγ 27.0(0.92);Cδ 24.6(0.10);Cδ 22.8(-0.10)
T15	109.1 (9.27)	174.1	58.0 (5.58)	72.7 (4.22)	Cγ 21.6(1.14)
Y16	115.0 (8.57)	171.4	54.9 (5.67)	43.1 (3.18,2.50)	Cδ - (7.59)
R17	117.0 (8.40)	173.6	54.7 (4.66)	34.3 (1.92,1.52)	Cγ 27.8(1.76,1.05);Cδ 44.1(2.95,2.81)
I18	126.1 (9.21)	174.9	60.9 (4.43)	37.0 (1.78)	Cγ 28.0(1.91,0.84);Cγm 17.1(0.27); Cδ 14.2(1.20)
E19	126.4 (9.77)	175.3	59.3 (3.91)	31.3 (2.20,2.06)	Cγ 37.7(2.34,2.17)
N20	112.4 (7.82)	169.7	51.5 (4.74)	39.1 (3.07)	Nδ 111.5(7.95,7.57)
Y21	111.9 (8.43)	173.8	58.2 (4.20)	40.7 (2.95,2.66)	Cδ 131.9(6.98);Cε 117.8(6.87)
T22	- (-)	173.2	55.6 (4.94)	66.7 (3.59)	Cγ 18.7(0.53)
P23	- (-)	176.9	62.6 (4.67)	31.3 (2.28,2.10)	Cγ 26.4(2.07);Cδ 50.1(3.91,3.71)
D24	119.6 (8.99)	175.2	55.6 (4.14)	41.0 (3.25,2.83)	
L25	114.5 (7.10)	172.8	51.0 (4.93)	47.3 (1.48,1.24)	Cγ 25.9(1.56);Cδ 26.2(0.63);Cδ 24.6(0.99)

P26	- (-)	177.4	62.1 (4.49)	32.1 (2.50,1.91)	Cγ 26.4(2.07); ;Cδ 50.1(3.91,3.71)
R27	123.5 (8.68)	177.9	60.0 (3.81)	29.6 (1.57,1.45)	Cγ 26.3(1.10);Cδ 43.1(2.69,2.60)
A28	115.0 (8.78)	180.0	54.7 (4.20)	18.2 (1.41)	
D29	114.2 (7.32)	179.3	57.0 (4.62)	41.0 (2.85,2.61)	
V30	121.4 (7.70)	176.9	66.4 (3.55)	31.1 (2.63)	Cγ 23.9(0.95);Cγ 21.6(1.00)
D31	116.2 (8.60)	179.3	57.9 (4.47)	40.0 (2.78)	
H32	115.6 (8.35)	176.0	58.9 (4.56)	29.6 (3.39,3.25)	Cδ 120.84(7.23)
A33	118.7 (8.13)	180.2	54.9 (4.03)	18.4 (1.54)	
I34	113.9 (7.97)	176.9	62.3 (3.67)	36.0 (2.28)	Cγ 28.3(1.64,1.32);Cγm 18.9(0.88); Cδ 9.7(0.55)
E35	119.3 (8.81)	179.6	60.1 (4.14)	29.6 (2.37,2.27)	Cγ 36.0(2.54,2.43)
K36	114.7 (8.60)	178.6	57.9 (4.08)	31.6 (1.46)	Cγ 24.7(1.32,1.27); Cδ 28.1(1.32,1.46) Cε 41.5(2.80,2.75)
A37	120.3 (7.57)	177.5	55.2 (4.00)	17.8 (1.38)	
F38	112.5 (7.81)	178.3	63.3 (3.82)	38.6 (2.71)	Cδ 130.4(5.72);Cε 129.4(5.94); Cζ 127.4 (6.52)
Q39	115.6 (8.01)	177.1	58.0 (4.28)	28.2 (2.30,2.26)	Cγ 33.8(2.64,2.54)
L40	114.5 (7.31)	178.5	57.3 (3.97)	41.7 (1.54,0.82)	Cγ 25.9(1.82);Cδ 25.9(0.64);Cδ 23.5(0.79)
W41	113.2 (6.78)	179.9	58.0 (4.74)	30.4 (3.27,3.15)	Cδ1 127.2(7.03);Nε1 123.0(9.45); Cζ2 114.7(7.28);Cη 124.1(6.81); Cζ3 121.4(6.89);Cε3 119.2 (7.45)
S42	114.3 (9.07)	175.8	60.9 (4.41)	63.2 (4.41,4.17)	
N43	113.9 (8.15)	176.7	54.8 (4.75)	38.9 (3.11,2.93)	
V44	102.5 (7.05)	174.5	60.0 (4.96)	32.4 (2.73)	Cγ 21.4(1.20), Cγ 18.6(1.00)
T45	108.4 (7.60)	172.8	59.6 (5.42)	71.9 (4.20)	Cγ 23.9(1.64)
P46	- (-)	176.2	62.0 (4.92)	31.5 (2.37,2.07)	Cγ 27.4(2.04,2.00);Cδ 51.4(3.57,3.32)
L47	114.8 (7.18)	176.8	54.7 (4.54)	43.1 (1.37,0.62)	Cγ 27.3(1.17);Cδ 25.6(0.42);Cδ 21.8(0.42)
T48	110.8 (8.30)	171.4	59.6 (4.39)	71.7 (4.01)	Cγ 21.2(1.10)
F49	116.3 (8.38)	175.6	55.7 (5.42)	41.7 (2.54,2.19)	Cδ 132.7(6.88);Cε 130.1(7.04); Cζ 133.0 (7.03)
T50	118.1 (8.61)	171.3	61.4 (4.50)	71.5 (3.75)	Cγ 21.3(1.18)
K51	127.3 (8.45)	176.0	55.4 (3.39)	33.1 (1.52,1.25)	Cγ 24.6(0.94,0.86);Cδ 29.8(1.78,1.62); Cε 42.0(3.04)
V52	120.4 (8.76)	175.7	59.4 (4.67)	33.9 (2.21)	Cγ 21.3(0.92);Cγ 19.7(0.79)
S53	114.0 (8.82)	173.1	58.7 (4.55)	64.0 (3.98,3.95)	
E54	115.8 (7.53)	174.3	54.4 (4.51)	32.6 (2.10,1.93)	Cγ 34.9(2.17)

G55	105.5 (8.56)	172.9	44.4 (4.11,3.82)		
Q56	116.2 (8.32)	174.4	55.1 (4.34)	29.1 (2.01)	Cγ 33.5(2.40)
A57	124.3 (7.73)	175.6	49.4 (4.56)	22.1 (1.01)	
D58	118.8 (8.13)	177.1	58.3 (4.48)	41.0 (2.87,2.25)	
I59	122.1 (8.82)	173.6	61.1 (4.26)	39.3 (1.99)	Cγ 27.1(1.56,1.48);Cγm 15.2(1.23); Cδ 14.1(1.00)
M60	124.3 (7.59)	176.6	52.8 (5.30)	31.7 (2.41,2.14)	Cγ 32.0(2.81,2.68); Cε 16.5(2.17)
I61	124.6 (9.27)	174.2	60.1 (5.62)	40.3 (1.97)	Cγ 28.7(1.90,1.16);Cγm 17.0(0.84); Cδ15.1(1.04)
S62	115.7 (8.65)	171.7	56.5 (5.09)	66.1 (3.94,3.68)	
F63	119.7 (9.18)	176.3	56.6 (5.31)	40.4 (3.09,2.78)	Cδ 133.3(7.05);Cε 131.8(6.25); Cζ 127.9 (6.32)
V64	114.5 (8.93)	173.3	58.7 (4.88)	36.7 (1.82)	Cγ 21.7(0.74);Cγ 16.7(0.07)
R65	115.4 (8.64)	175.7	53.9 (5.25)	33.9 (1.88,1.75)	Cγ 26.4(1.62,1.58);Cδ 43.1(3.34,3.26)
G66	105.2 (9.35)	175.6	46.5 (3.95,3.82)		
D67	126.9 (9.27)	174.9	54.8 (4.55)	40.1 (3.02,2.72)	
H68	122.4 (9.35)	173.3	53.6 (5.11)	26.5 (3.45,2.73)	Cδ 127.6(6.58);Cε 139.7(7.41)
R69	109.3 (8.18)	175.2	57.8 (3.97)	26.1 (2.20,2.07)	Cγ 27.2(1.55);Cδ 42.9(3.24)
D70	113.6 (7.18)	175.8	52.0 (4.71)	40.4 (3.18,2.72)	
N71	111.4 (8.20)	174.3	53.7 (4.52)	37.7 (2.97)	
S72	112.6 (7.63)	174.1	54.2 (4.70)	63.6 (3.23,2.94)	
P73	- (-)	179.2	62.7 (4.54)	31.5 (2.34,1.98)	Cγ 27.4(2.05,1.95);Cδ 49.3(3.56,3.29)
F74	117.9 (8.23)	175.9	58.3 (5.03)	39.5 (4.05,2.99)	Cδ - (7.09);Cε - (6.23);Cζ - (6.56)
D75	113.6 (8.53)	177.0	53.3 (4.72)	40.9 (3.21,2.80)	
G76	108.1 (8.84)	170.2	44.0 (4.49)		
P77	- (-)	177.9	63.5 (4.06)	31.2 (2.31,1.89)	Cγ 24.5(2.01,1.87);Cδ -(3.72,3.50)
G78	117.2 (11.42)	174.1	43.0 (4.24,3.56)		
G79	108.0 (8.60)	175.1	46.2 (4.00,3.50)		
N80	126.6 (11.05)	175.4	54.0 (4.67)	38.6 (3.03,2.94)	Nδ 112.0(7.67,7.12)
L81	122.7 (9.23)	175.2	55.6 (4.51)	43.6 (1.68,1.46)	Cγ 25.7(1.60);Cδ 20.3(-0.22);Cδ 25.6(0.32)
A82	112.0 (7.47)	174.7	51.0 (4.75)	21.4 (1.10)	
H83	109.8 (8.82)	171.8	54.2 (4.85)	30.5 (3.44,2.93)	Cδ -(6.40);Cε 140.8(7.98)
A84	118.0 (7.93)	175.6	50.4 (5.16)	23.6 (1.36)	
F85	117.9 (8.19)	174.8	56.9 (4.39)	41.1 (3.11,3.06)	Cδ 132.2(7.10);Cε 130.1(6.78); Cζ 129.0 (6.89)
Q86	116.0 (8.28)	173.9	54.1 (4.36)	26.6 (2.04,1.81)	Cγ 33.3(2.40)

P87	- (-)	173.5	64.4 (2.94)	31.6 (0.69,-0.12)	Cδ 49.2(3.56,3.29)
G88	105.2 (5.68)	169.1	43.9 (4.23,3.71)		
P89	- (-)	178.1	62.2 (4.69)	32.8 (2.45,2.08)	Cγ 26.5(2.10,2.00);Cδ 48.9(3.57)
G90	108.8 (9.01)	174.7	47.0 (4.03,3.78)		
I91	132.4 (9.09)	173.9	61.4 (4.28)	38.1 (1.53)	Cγ 27.9(1.00,0.52);Cγm 16.1(0.52); Cδ 14.5(0.52)
G92	104.1 (7.68)	174.8	46.5 (3.30,3.82)		
G93	116.5 (7.65)	171.7	46.5 (4.78,4.29)		
D94	120.5 (8.36)	173.6	55.7 (4.75)	39.8 (3.13,3.04)	
A95	116.5 (8.42)	174.4	50.6 (4.96)	21.1 (1.06)	
H96	118.6 (9.03)	172.9	50.6 (5.58)	33.5 (2.52,2.91)	Cδ 117.2(7.25);Cε 141.1(8.46)
F97	119.7 (8.90)	173.9	56.2 (4.28)	41.1 (2.25,1.96)	Cδ 131.8(6.25);Cε 128.7(6.59); Cζ 125.4 (6.49)
D98	120.1 (8.08)	179.1	53.8 (4.37)	39.9 (3.00,0.58)	
E99	128.9 (9.93)	176.6	56.0 (4.55)	30.9 (2.11,1.78)	Cγ 36.2(2.75,2.41)
D100	116.1 (8.90)	176.5	56.2 (4.73)	38.9 (2.70,2.34)	
E101	113.3 (7.45)	175.6	52.9 (4.71)	27.2 (1.23,0.63)	Cγ 34.8(2.57,1.79)
R102	123.8 (7.97)	173.1	54.3 (4.43)	28.9 (1.84,1.47)	Cγ 26.2(1.59,1.16);Cδ 42.6(3.09,3.02)
W103	127.8 (9.27)	177.1	55.4 (5.50)	30.8 (3.22,3.11)	Cδ1 -(7.41);Nε1 123.6(9.46);Cζ2 -(7.28) Cη 123.1(7.03);Cζ3 119.9(6.87); Cε3 121.8 (7.62)
T104	109.9 (9.32)	174.8	59.6 (4.85)	71.3 (4.34)	Cγ 20.2(0.73)
N105	115.2 (8.42)	174.5	50.9 (5.06)	38.7 (3.13,2.70)	
N106	116.7 (7.88)	173.3	52.1 (4.94)	38.0 (3.33,3.01)	Nδ 110.10(7.57,6.75)
F107	110.1 (7.57)	177.2	58.2 (4.46)	38.5 (2.63,2.67)	Cδ 131.5(7.00);Cε 130.7(7.23); Cζ 129.9 (7.12)
R108	121.2 (8.03)	175.0	55.8 (4.06)	29.7 (1.83,1.67)	Cγ 27.4(1.45,1.35);Cδ 43.1(3.13)
E109	119.0 (8.56)	177.9	52.3 (3.79)	27.4 (1.16,-0.05)	Cγ 36.6(2.19,1.97)
Y110	122.1 (8.28)	173.2	61.9 (3.80)	41.2 (2.27,1.99)	Cδ 137.8(5.68);Cε 118.5(6.47)
N111	121.5 (8.45)	175.7	54.7 (4.89)	39.2 (2.26)	
L112	127.7 (9.02)	176.9	58.0 (4.48)	41.2 (1.96,1.64)	Cγ 27.2(1.20);Cδ 27.8(0.78);Cδ 21.8(-0.04)
H113	117.7 (9.05)	175.7	59.9 (4.09)	27.9 (3.79,3.19)	Cδ -(7.90);Cε -(8.06)
R114	115.2 (8.91)	178.5	58.0 (3.96)	29.1 (2.41)	Cγ 26.0(1.83); Cδ 42.0(3.59,3.42)
V115	116.8 (8.18)	178.1	66.8 (4.05)	32.1 (2.51)	Cγ 24.5(1.65);Cγ 22.3(1.36)
A116	121.2 (10.00)	178.0	55.6 (4.01)	17.5 (1.21)	
A117	115.5 (8.57)	177.9	56.4 (3.84)	18.5 (1.20)	

H118	111.1 (7.01)	175.9	58.7 (4.40)	28.2 (3.86,3.08)	Cδ 127.0(6.85);Cε 137.1(7.89)
E119	113.5 (8.94)	177.8	57.8 (4.08)	26.8 (1.97,1.75)	Cγ 31.7(2.93)
L120	113.9 (8.67)	177.7	56.0 (4.06)	40.1 (1.42,0.77)	Cγ 26.3(1.52);Cδ 22.8(-0.42);Cδ 21.2(0.37)
G121	103.1 (7.22)	177.5	47.6 (3.89,2.44)		
H122	117.7 (7.02)	179.3	57.5 (5.01)	27.2 (3.75,2.73)	Cδ 127.5(6.98);Cε 137.8(6.70)
S123	115.4 (8.06)	174.6	62.6 (4.33)	- (4.69)	
L124	111.7 (7.17)	177.6	54.5 (4.59)	42.3 (1.73,1.60)	Cγ 25.6(2.06);Cδ 24.2(0.42);Cδ 22.0(0.94)
G125	105.8 (8.23)	173.8	44.3 (4.77,3.61)		
L126	117.5 (8.36)	177.4	54.5 (4.56)	42.1 (1.60,1.21)	Cγ 26.5(1.45);Cδ 27.1(0.91);Cδ 21.9(0.82)
S127	115.8 (8.58)	173.4	56.3 (4.70)	64.5 (4.01,3.94)	
H128	114.4 (8.48)	174.4	56.4 (5.18)	29.2 (2.97,2.31)	Cδ 125.5(7.36)
S129	112.7 (7.12)	175.5	54.9 (4.86)	64.7 (4.34,3.31)	
T130	112.3 (8.65)	174.0	61.7 (4.62)	68.8 (4.68)	Cγ 21.3(1.36)
D131	123.2 (8.85)	175.9	53.5 (4.64)	41.1 (2.96,2.46)	
I132	122.8 (7.95)	176.3	62.5 (2.62)	38.2 (1.45)	Cγ 27.5(1.09,1.03);Cγm 16.6(0.75); Cδ 13.9(0.75)
G133	107.2 (8.65)	173.7	44.3 (4.17,3.57)		
A134	121.5 (8.07)	179.2	51.3 (4.58)	18.8 (1.87)	
L135	130.6 (12.26)	180.9	57.5 (4.34)	41.3 (1.75,1.65)	Cγ 26.8(1.77);Cδ 25.9(0.69);Cδ 23.9(0.92)
M136	110.0 (8.55)	177.5	53.2 (4.85)	26.9 (2.45)	Cγ 29.9(2.86,2.72);Cε 11.5(0.60)
Y137	126.5 (8.12)	176.5	57.7 (4.95)	38.7 (3.84,3.00)	Cδ 134.1(7.13);Cε 117.7(6.78)
P138	- (-)	175.2	64.1 (3.68)	29.1 (1.78)	Cγ 26.9(1.44);Cδ 50.3(3.47,2.16)
S139	110.9 (7.07)	173.7	57.7 (4.54)	64.4 (3.96,3.92)	
Y140	124.1 (9.19)	174.4	60.1 (4.38)	38.4 (3.20,2.99)	Cδ 133.4(7.25);Cε 117.7(7.06)
T141	117.8 (6.68)	173.6	60.0 (4.20)	71.7 (4.11)	Cγ 21.3(1.22)
F142	- (-)	178.7	58.0 (4.47)	38.4 (3.27)	Cδ - (7.37)
S143	- (-)	173.8	56.7 (4.56)	63.8(4.01,3.76)	
G144	- (-)	171.8	45.5 (4.36,2.93)		
D145	118.2 (7.63)	174.4	52.8 (4.81)	42.5 (2.51)	
V146	121.2 (8.60)	173.5	62.1 (4.19)	32.1 (2.20)	Cγ 21.8(0.61);Cγ 22.3(1.04)
Q147	122.0 (8.39)	174.3	53.0 (4.58)	32.2 (2.06,1.73)	Cγ 32.4(2.24)
L148	117.3 (8.56)	177.2	54.7 (4.15)	41.5 (1.61,1.43)	Cγ 26.2(1.25);Cδ 26.9(0.43);Cδ 22.0(-0.23)
A149	124.3 (9.94)	178.2	49.7 (4.74)	20.8 (1.63)	
Q150	120.8 (9.10)	177.5	59.0 (3.82)	27.3 (2.26,2.08)	Cγ 33.0(2.56,2.48)
D151	112.8 (8.78)	178.7	58.2 (4.44)	43.9 (2.95,2.30)	
D152	112.6 (7.09)	177.3	57.0 (4.83)	44.1 (3.09,2.99)	

I153	117.6 (7.93)	177.5	65.5 (3.64)	38.3 (1.88)	Cγ 30.1(1.82);Cγm 16.5(0.96); Cδ 12.6(0.83)
D154	117.0 (9.24)	180.0	57.0 (4.46)	39.6 (2.81,2.78)	
G155	104.8 (8.10)	176.0	47.1 (4.08,3.97)		
I156	119.8 (8.64)	178.1	60.8 (4.66)	38.7 (2.32)	Cγ 30.9(1.81,2.03);Cγm 20.3(1.67); Cδ 15.2(1.06)
Q157	121.5 (8.85)	179.5	58.0 (4.45)	27.1 (2.36,1.79)	Cγ 34.4(2.88,3.07)
A158	120.3 (7.97)	178.1	54.3 (4.20)	17.7 (1.62)	
I159	112.0 (7.01)	177.2	63.6 (3.84)	39.6 (1.61)	Cγ 26.7(1.87);Cγm 17.6(0.12); Cδ 13.8(0.87)
Y160	110.9 (7.78)	175.5	59.7 (4.62)	40.7 (3.42,2.77)	Cδ 133.4(7.39);Cε 118.0(7.39)
G161	106.7 (8.35)	171.7	43.7 (4.47,3.96)		
R162	111.6 (7.94)	176.6	54.9 (4.76)	31.9 (1.87,1.77)	Cγ 26.8(1.63);Cδ 43.4(3.25)
S163	111.7 (7.51)	174.3	58.1 (4.13)	63.3 (3.81,3.73)	
Q164	119.8 (8.64)	175.0	55.3 (4.41)	29.2 (2.18,1.98)	Cγ 33.5(2.41)
N165	118.6 (8.44)	172.9	51.1 (5.02)	38.6 (2.88,2.71)	
P166	- (-)	176.4	62.9 (4.52)	32.0 (2.33,1.96)	Cγ 26.9(2.04);Cδ 50.4(3.81)
V167	118.3 (8.19)	175.5	62.0 (4.11)	32.4 (2.08)	Cγ 20.7(0.98);Cγ 20.4(1.02)
Q168	123.5 (8.36)	175.7	52.9 (4.71)	29.0 (2.18,2.02)	Cγ 33.3(2.45)
P169	- (-)	181.0	64.4 (4.41)	33.9(2.35,2.17)	Cγ 24.6(1.96,1.89);Cδ 49.5(3.65,3.49)

Footnotes to Table 1

[a]In each column, ^{15}N and ^{13}C shifts are listed first, and the corresponding ^{1}H shifts are given in parentheses. ^{1}H and ^{13}C chemical shifts are reported relative to 3-(trimethylsily)propionic-d_4 acid and ^{15}N shifts relative to external liguid NH_3.