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Table S1

Residue	¹⁵ N	CO	C α	C β	others
A1	-	-	51.23(4.60)	20.03(1.25)	
S2	-	-	57.55(4.53)	61.22(3.12)	
S3	-	174.11	57.87(4.42)	63.69(3.99)	
G4	110.81(8.16)	-	44.55(4.23,4.10)		
P5	-	176.49	62.72(4.46)	31.78(2.25,1.99)	C γ H2:26.92(2.01);C δ H2:49.63(3.69,3.62)
A6	124.24(8.29)	177.61	52.03(4.43)	20.17(1.53)	
G7	107.47(8.29)	-	45.65(3.77,4.00)		
C8	115.78(8.23)	176.58	54.47(5.45)	52.60(3.81,2.59)	
Q9	120.94(8.72)	173.99	54.01(5.26)	33.25(2.12,1.79)	C γ H2:32.56(1.78);C δ :178.83;N ϵ 2H2:110.54(7.24,6.68)
V10	126.10(8.70)	173.63	60.44(4.69)	33.97(1.12)	C γ H3:22.40(0.46);C γ' H3:19.86(-0.17)
L11	127.32(8.78)	174.13	54.47(4.66)	42.09(1.56,1.46)	C γ H:27.65(1.38);C δ' H3:24.42(0.75);C δ'' H3:24.07(0.72)
W12	128.02(8.64)	173.73	55.97(4.47)	30.56(3.29,2.56)	C δ 1H:126.86(7.08);C ζ 2H:112.99(7.44);C η 2H:123.01(7.15); C ζ 3H:119.45(6.41);C ϵ 3H:120.44(7.03);N ϵ 1H:130.16(10.13)
G13	116.51(7.65)	171.77	44.54(4.43,3.48)		
V14	120.35(8.23)	174.36	59.52(5.12)	35.71(1.75)	C γ H3:21.23(0.74);C γ' H3:21.23(0.75)
N15	123.75(8.52)	173.24	52.75(4.93)	41.55(2.43,2.35)	C γ :176.30;N δ 2H2:112.15(7.54,6.97)
Q16	122.56(9.01)	173.23	55.18(4.90)	33.06(2.02,1.86)	C γ H2:33.62(2.45,2.15);C δ :179.22;N ϵ 2H2:112.12(7.40,6.63)
W17	124.30(8.45)	-	56.60(5.28)	29.59(3.67,3.47)	C δ 1H:125.33(7.39);C ζ 2H:113.18(6.96);C η 2H:118.77(6.82); C ζ 3H:121.00(7.09);C ϵ 3H:120.13(7.31);N ϵ 1H:130.25(9.71)
N18	-	176.09	57.35(4.54)	37.03(3.20,3.12)	C γ -;N δ 2H2:-(-,-)
T19	104.95(7.26)	173.68	60.03(4.04)	69.60(4.56)	C γ 2H3:21.25(1.13)
G20	109.57(6.03)	168.70	45.91(4.11,3.42)		
P21	115.66(7.69)	171.33	56.02(4.50)	40.78(2.81,2.70)	C δ H:131.48(6.67);C ϵ H:129.95(7.25);C ζ H:127.45(7.25)
T22	117.41(8.98)	172.77	61.20(5.11)	71.78(4.03)	C γ 2H3:22.08(1.40)
A23	130.96(9.11)	174.17	49.28(4.76)	19.81(-0.19)	
N24	121.02(8.46)	173.32	52.71(4.65)	40.59(2.47,2.41)	C γ :176.69;N δ 2H2:112.15(7.50,6.66)
V25	126.82(8.41)	174.19	60.51(4.45)	32.69(0.23)	C γ H3:22.54(0.48);C γ' H3:21.57(0.12)
T26	122.48(8.33)	172.70	61.22(4.85)	70.22(3.89)	C γ 2H3:21.16(1.07)
V27	126.88(9.17)	173.04	60.29(4.37)	33.94(1.56)	C γ H3:21.37(0.57);C γ' H3:21.48(0.46)
K28	126.80(9.32)	175.52	53.79(4.99)	35.35(1.78,1.39)	C γ H2:24.72(1.12,0.92);C δ H2:29.12(1.41);C ϵ H2:41.54(2.69)
N29	123.02(8.36)	174.63	51.14(4.77)	38.23(3.23,3.15)	C γ :175.83;N δ 2H2:112.16(8.38,6.62)
T30	116.59(7.46)	173.97	60.42(4.45)	66.76(4.42)	C γ 2H3:22.12(0.93)
S31	119.78(7.91)	172.47	57.46(4.76)	64.37(4.30,4.14)	
S32	112.00(8.18)	173.22	57.92(4.43)	64.72(4.02,3.88)	
A33	127.30(8.40)	-	48.87(4.99)	20.34(1.37)	
P34	-	175.68	62.35(4.31)	32.32(2.28,1.85)	C γ H2:26.59(2.04,1.97);C δ H2:50.13(3.83,3.73)
V35	122.80(8.13)	174.61	61.40(4.13)	34.30(1.96)	C γ H3:21.21(0.92);C γ' H3:22.16(1.01)
D36	130.04(8.84)	174.52	53.55(4.99)	41.27(2.69,2.33)	
G37	115.34(8.44)	172.44	44.32(4.31,3.28)		
W38	120.47(8.44)	174.17	54.70(5.60)	31.75(3.15,3.03)	C δ 1H:126.60(7.23);C ζ 2H:111.95(7.03);C η 2H:122.89(6.35); C ζ 3H:119.70(6.25);C ϵ 3H:121.98(7.11);N ϵ 1H:130.70(10.32)
T39	114.53(8.18)	173.58	60.42(5.33)	71.30(3.99)	C γ 2H3:21.70(1.03)
L40	132.92(10.32)	172.29	52.74(5.93)	46.04(2.18,1.52)	C γ H:27.73(1.94);C δ' H3:26.94(1.18);C δ'' H3:25.05(1.03)
T41	117.46(9.40)	173.80	58.79(5.52)	71.22(4.31)	C γ 2H3:22.25(1.17)
F42	115.86(7.94)	172.06	56.33(4.61)	40.11(3.23,2.25)	C δ H:131.79(6.54);C ϵ H:129.27(6.54);C ζ H:129.80(7.03)
S43	115.41(8.93)	174.71	56.02(5.43)	64.85(3.57,3.45)	

F44	125.05(9.21)	-	56.04(4.93)	39.55(3.71,2.88)	C ₆ H:132.10(7.27);C ₆ H:129.18(7.56);C ₇ H:128.04(7.63)
P45	-	178.08	63.58(4.74)	32.60(2.30,1.95)	C ₇ H ₂ :27.33(2.02,1.82);C ₈ H ₂ :51.11(3.98)
S46	112.69(7.96)	175.29	56.70(4.86)	63.96(3.82,3.55)	
G47	110.24(8.92)	175.40	45.21(4.11,3.60)		
Q48	121.16(9.10)	174.79	57.57(4.24)	26.23(1.47,0.07)	C ₇ H ₂ :(-2.24,2.19);C ₈ :179.96;N ₂ H ₂ :114.75(8.10,7.04)
Q49	116.92(7.64)	174.97	53.66(4.99)	31.84(1.94,1.81)	C ₇ H ₂ :33.32(2.29,2.29);C ₈ :179.83;N ₂ H ₂ :111.29(7.09,6.67)
V50	123.12(8.65)	176.30	63.96(4.04)	31.92(1.93)	C ₇ H ₃ :20.95(0.77);C ₇ 'H ₃ :20.95(0.70)
T51	120.69(9.47)	174.72	62.50(4.60)	69.59(4.32)	C ₇ H ₃ :22.55(1.33)
Q52	121.32(7.59)	172.41	56.14(4.59)	31.74(2.35,2.11)	C ₇ H ₂ :33.73(2.44);C ₈ :179.83;N ₂ H ₂ :111.30(7.68,7.15)
A53	126.62(8.82)	175.96	50.93(4.85)	24.15(1.35)	
W54	117.17(8.24)	176.12	55.94(5.36)	30.85(3.37,3.28)	C ₈ H:125.19(7.04);C ₇ H ₂ :112.88(6.93);C ₇ H ₂ :121.25(6.64); C ₇ H ₃ :124.74(6.80);C ₈ H ₃ :123.80(6.91);N ₂ H ₂ :129.05(9.56)
S55	114.47(9.78)	170.17	59.41(4.07)	62.69(4.72,4.58)	
S56	103.75(7.54)	173.60	57.54(4.35)	63.57(3.86,3.11)	
T57	113.05(8.26)	173.30	61.64(4.42)	70.15(3.69)	C ₇ H ₃ :21.54(1.06)
V58	127.28(8.74)	174.70	61.05(4.79)	33.62(1.61)	C ₇ H ₃ :23.13(0.71);C ₇ 'H ₃ :22.41(0.54)
T59	120.96(8.77)	-	60.32(4.51)	70.89(3.98)	C ₇ H ₃ :20.80(1.07)
Q60	-	174.42	54.18(5.11)	29.66(1.86,1.69)	C ₇ H ₂ :32.88(2.40,2.13);C ₈ :178.28;N ₂ H ₂ :107.22(7.79,7.24)
S61	122.86(8.67)	-	55.88(4.68)	63.07(3.77,3.60)	
G62	-	-	45.21(4.11,3.72)		
S63	-	172.86	58.22(4.87)	64.17(4.49,4.02)	
A64	125.11(7.90)	176.11	52.38(4.40)	19.35(1.43)	
V65	127.32(8.82)	174.57	61.42(4.18)	32.43(-0.02)	C ₇ H ₃ :23.44(0.24);C ₇ 'H ₃ :22.82(0.18)
T66	123.26(8.56)	172.48	61.73(4.59)	70.10(3.80)	C ₇ H ₃ :20.86(0.94)
V67	129.08(9.54)	173.24	60.37(4.59)	33.52(2.23)	C ₇ H ₃ :20.95(1.02);C ₇ 'H ₃ :20.96(0.22)
R68	126.00(8.67)	174.71	53.35(4.82)	33.44(1.53,1.26)	C ₇ H ₂ :27.71(1.55,1.38);C ₈ H ₂ :42.98(3.05)
N69	114.91(6.29)	174.97	54.82(2.95)	38.42(2.28,0.02)	C ₇ :176.15;N ₂ H ₂ :116.91(7.11,6.60)
A70	124.04(8.11)	-	49.71(4.08)	15.08(-0.13)	
P71	-	176.88	65.25(4.07)	31.44(2.42,1.96)	C ₇ H ₂ :24.63(2.18,1.90);C ₈ H ₂ :49.80(3.42,3.04)
W72	107.72(6.13)	176.33	56.33(4.90)	28.36(3.42,3.09)	C ₈ H:126.07(6.87);C ₇ H ₂ :113.69(7.61);C ₇ H ₂ :124.40(7.43); C ₇ H ₃ :121.99(7.29);C ₈ H ₃ :119.34(7.53);N ₂ H ₂ :130.61(9.97)
N73	121.24(7.25)	175.21	51.76(5.35)	38.25(3.60,2.71)	C ₇ :175.66;N ₂ H ₂ :105.40(7.66,7.29)
G74	105.36(7.98)	173.70	47.26(3.82,3.67)		
S75	115.16(7.97)	174.70	56.82(5.32)	62.91(3.88,3.81)	
I76	126.02(8.90)	-	58.30(4.67)	39.38(1.75)	C ₇ H ₂ :25.42(1.49,0.68);C ₈ H ₃ :19.28(0.77);C ₇ H ₃ :12.89(0.10)
P77	-	175.93	62.34(4.33)	32.24(2.42,1.85)	C ₇ H ₂ :26.58(2.05,1.98);C ₈ H ₂ :51.19(3.86,3.75)
A78	125.50(8.68)	178.63	54.37(3.78)	17.68(1.13)	
G79	115.54(8.27)	173.95	46.07(4.12,3.74)		
G80	108.89(8.59)	171.97	43.74(4.49,3.58)		
T81	106.05(8.03)	174.18	59.07(5.65)	73.68(3.94)	C ₇ H ₃ :21.55(0.99)
A82	121.86(8.87)	175.34	51.31(4.89)	22.35(1.41)	
Q83	119.16(8.82)	174.54	54.41(5.60)	32.82(2.17,2.03)	C ₇ H ₂ :34.45(2.47,2.31);C ₈ :180.50;N ₂ H ₂ :111.39(7.35,6.84)
F84	118.76(8.54)	171.10	55.93(4.91)	40.15(3.40,3.23)	C ₈ H:132.20(7.03);C ₆ H:127.75(7.03);C ₇ H:128.14(7.16)
G85	107.51(8.29)	168.70	45.65(3.82,3.64)		
F86	110.60(7.44)	172.89	55.85(4.03)	40.28(3.24,3.15)	C ₈ H:132.10(6.94);C ₆ H:129.18(7.38);C ₇ H:128.04(7.77)
N87	117.42(9.02)	175.61	50.83(5.80)	41.37(2.97,2.82)	C ₇ :176.30;N ₂ H ₂ :110.47(7.59,7.10)
G88	107.82(8.38)	172.01	45.37(5.00,3.28)		
S89	116.15(9.34)	172.87	55.97(5.05)	66.17(3.96,3.72)	

H90	116.98(7.38)	174.13	54.80(4.90)	33.74(3.24,2.45)	C δ 2H:114.16(6.07);C ϵ 1H:138.93(7.48)
T91	111.04(9.22)	175.22	60.56(4.44)	68.67(4.68)	C γ 2H3:21.20(1.15)
G92	117.68(10.63)	174.22	45.30(4.74,3.58)		
T93	116.60(7.73)	-	61.24(4.13)	70.26(3.94)	C γ 2H3:20.90(1.15)
N94	-	172.30	50.18(4.58)	37.02(2.33,1.04)	C γ :176.41;N δ 2H2:105.49(7.21,3.99)
A95	125.58(7.36)	176.13	51.71(4.13)	18.11(1.18)	
A96	124.30(8.01)	-	49.91(4.12)	16.81(0.95)	
P97	-	175.45	61.97(4.17)	30.50(1.95,0.60)	C γ H2:28.63(1.12,0.52);C δ H2:49.70(3.22,1.49)
T98	108.31(8.07)	173.52	60.54(4.11)	69.73(4.34)	C γ 2H3:21.64(1.10)
A99	122.57(6.82)	174.84	51.54(4.52)	20.48(1.57)	
F100	119.22(8.66)	175.09	56.38(5.28)	44.95(2.80,2.38)	C δ H:131.10(6.84);C ϵ H:129.62(6.39);C ζ H:128.53(5.97)
S101	116.72(8.72)	172.06	56.91(5.47)	65.38(3.55,3.36)	
L102	128.29(8.92)	175.84	53.12(5.37)	45.79(2.35)	C γ H:27.73(1.37);C δ 'H3:25.82(0.83);C δ ''H3:25.73(0.69)
N103	127.55(9.82)	175.21	53.98(4.52)	36.96(3.24,3.11)	C γ :177.95;N δ 2H2:109.87(7.96,7.21)
G104	102.33(8.30)	173.78	44.86(4.23,3.52)		
T105	120.97(8.08)	-	59.75(4.71)	70.68(4.30)	C γ 2H3:20.89(1.24)
P106	-	-	63.00(4.74)	34.09(2.35,2.03)	C γ H2:27.37(2.21,1.98);C δ H2:51.08(4.04,3.80)
C107	- (8.77)	176.77	51.55(5.36)	41.13(3.07,2.69)	
T108	115.18(8.57)	173.31	61.80(4.54)	69.79(4.25)	C γ 2H3:22.23(1.15)
V109	122.20(8.41)	175.92	61.59(4.71)	32.98(2.07)	C γ 'H3:21.32(1.02);C γ ''H3:21.39(1.00)
G110	121.75(8.45)	-	45.83(3.88,3.47)		