SUPPLEMENTARY MATERIAL for $^1$H, $^{15}$N, $^{13}$C, and $^{13}$CO Assignments and Secondary Structure Determination of Collagenase-3 (MMP-13) Complexed with a Hydroxamic Acid Inhibitor by Franklin J. Moy, Pranab K. Chanda, Scott Cosmi, Wade Edris, Jeremy I. Levin and Robert Powers

<u>Table S1</u>  $^{15}$N, $^{13}$C, $^{13}$CO and $^1$H resonance assignments for MMP-13:WAY151693 at pH 6.5 and 35ºC.[a]

| Residue | N | CO | Cα | Cβ | Others |
|---------|---|----|----|----|--------|
| Y1 | -(-) | 171.7 | 55.6(4.32) | 38.1(3.32,3.09) | Cδ 129.7(6.84) |
| N2 | 119.0(9.80) | 173.3 | 53.4(5.07) | 43.3(2.50) | |
| V3 | 115.5(8.40) | 176.4 | 59.8(4.75) | 32.5(2.76) | Cγ 19.0(1.27);Cγ 18.6(1.04) |
| F4 | 121.4(8.04) | - | 58.7(4.32) | 43.3(3.87) | Cδ -(7.27) |
| P5 | -(-) | 177.2 | 64.3(4.41) | 31.7(1.93,2.38) | Cγ 28.1(2.19);Cδ 49.3(3.70,3.48) |
| R6 | 116.1(8.48) | 175.8 | 57.7(4.00) | 28.1(1.63) | Cγ 32.9(1.64);Cδ 43.4(3.25) |
| T7 | 114.3(8.41) | 173.8 | 62.6(3.87) | 67.5(4.32) | Cγ 22.7(1.24) |
| L8 | 122.7(6.89) | 175.8 | 54.7(4.29) | 42.2(1.62,1.36) | Cγ 26.5(1.71);Cδ 25.7(0.82);Cδ 22.7(0.82) |
| K9 | 116.6(7.85) | 175.6 | 55.0(4.50) | 34.6(1.84) | Cγ 22.9(1.47,1.19);Cδ 29.7(1.56,1.47); Cε 42.0(2.96) |
| W10 | 122.8(8.20) | - | 57.9(4.60) | 30.4(3.61,3.29) | Cδ1 -(7.37);Nε1 128.8(10.73); Cε3 121.6(7.88);Cζ3 121.7(7.09); Cζ2 112.6(7.40);Cη2 124.9(7.53) |
| S11 | -(-) | 172.8 | 58.4(4.65) | 63.5(4.21,4.08) | |
| K12 | 119.0(7.52) | 173.5 | 54.1(4.75) | 34.5(1.93,2.89) | Cγ 23.6(1.44,1.28);Cδ 29.7(1.96,1.75); Cε 42.4(2.99) |
| M13 | 114.0(8.19) | 174.4 | 54.3(4.50) | 33.9(2.11,1.90) | Cγ 33.3(2.77,2.54);Cε 19.0(2.20) |
| N14 | 115.8(7.36) | 173.4 | 51.8(4.87) | 37.9(2.63,2.57) | |
| L15 | 124.6(8.05) | 177.3 | 53.2(4.53) | 44.9(0.84,1.26) | Cγ 27.7(0.89);Cδ 25.0(0.01); Cδ 23.2(-0.18) |
| T16 | 112.5(9.39) | 174.2 | 58.1(5.57) | 72.9(4.11) | Cγ 21.9(1.14) |
| Y17 | 117.5(8.65) | 172.0 | 54.8(5.64) | 42.6(2.93,2.33) | Cδ -(6.32) |
| R18 | 119.4(8.24) | 173.5 | 55.1(4.54) | 34.3(1.86) | Cγ 28.4(1.73);Cδ 44.5(2.97,2.70) |
| I19 | 128.6(8.83) | 174.9 | 61.3(4.17) | 37.4(1.76) | Cγ 36.8(1.36);Cγm 17.6(0.39);Cδ -(1.01) |
| V20 | 130.2(9.66) | 175.5 | 66.5(3.48) | 32.2(2.25) | Cγ 23.5(1.11);Cγ 21.0(-) |
| N21 | 115.5(7.78) | 182.0 | 51.3(4.71) | 39.2(3.24,3.16) | |
| Y22 | 111.7(8.16) | 175.4 | 57.6(4.45) | 41.2(2.85,2.52) | Cδ 132.5(6.92);Cε -(6.84) |
| T23 | 110.8(7.61) | - | 55.2(4.98) | 67.5(2.97) | Cγ 19.7(0.61) |
| P24 | -(-) | 177.4 | 63.2(4.75) | 31.7(2.28,2.14) | Cγ 26.8(2.04);Cδ 51.4(4.51,3.65) |
| D25 | 121.8(8.94) | 175.6 | 56.0(4.17) | 41.7(3.40,2.78) | |
| M26 | 114.3(7.24) | 174.8 | 53.5(4.76) | 40.6(2.41,1.46) | Cγ 32.1(2.56,2.24);Cε 16.7(1.82) |
| T27 | 110.3(8.58) | - | 61.6(4.44) | 70.4(4.71) | Cγ 22.0(1.40) |
| H28 | -(-) | 177.8 | 58.8(4.26) | 28.4(3.04,2.85) | Cδ2 118.0(7.05) |

| Residue | N (H) | C' | Cα (Hα) | Cβ (Hβ) | Side chain |
|---|---|---|---|---|---|
| S29 | 112.5(8.59) | 177.3 | 61.3(4.38) | 62.5(3.97) | |
| E30 | 121.8(7.72) | 179.9 | 59.5(4.02) | 30.3(2.07,2.34) | Cγ 37.7(2.50,2.28) |
| V31 | 122.5(8.09) | 176.7 | 66.9(3.23) | 32.0(2.50) | Cγ 25.0(1.06);Cγ 23.3(0.90) |
| E32 | 117.5(8.51) | 180.0 | 59.9(4.01) | 29.1(2.44,2.17) | Cγ 37.3(2.89,2.52) |
| K33 | 119.8(8.44) | 178.3 | 59.3(4.09) | 32.9(1.96) | Cγ 25.3(1.64);Cδ 29.4(1.88,1.77); Cε 42.1(3.17) |
| A34 | 122.6(7.84) | 180.1 | 55.6(4.20) | 17.7(1.25) | |
| F35 | 113.8(7.93) | 177.3 | 58.8(4.68) | 37.2(3.12) | Cδ 129.6(7.02);Cε 131.2(6.67); Cζ 129.8(6.16) |
| K36 | 120.0(8.49) | 180.0 | 60.8(4.18) | 33.0(2.17) | Cγ 25.2(1.80,1.64);Cδ 32.8(1.92); Cε 42.1(3.19) |
| K37 | 119.8(8.44) | 178.7 | 59.8(4.08) | 32.8(1.91,1.80) | Cγ 25.4(1.63,1.30);Cδ 29.3(1.47,1.15); Cε 41.5(2.43) |
| A38 | 123.4(8.38) | 178.3 | 55.7(4.25) | 19.3(1.51) | |
| F39 | 114.3(8.12) | 178.4 | 63.0(4.22) | 38.8(2.55,2.67) | Cδ 129.7(5.67);Cε 128.7(5.32); Cζ 126.6(5.48) |
| K40 | 120.8(7.85) | 177.5 | 58.3(4.62) | 32.8(2.18,2.01) | Cγ 25.4(1.73,1.50);Cδ 29.8(1.88,1.76); Cε 42.4(3.22) |
| V41 | 112.9(7.35) | 176.8 | 65.1(3.96) | 31.2(2.08) | Cγ 22.7(0.73);Cγ 21.4(0.83) |
| W42 | 116.2(6.86) | 180.6 | 57.7(4.92) | 30.9(3.35) | Cδ1 127.8(7.48);Nε1 127.8(10.18); Cε3 119.3(7.52);Cζ3 121.9(6.99); Cζ2 115.7(7.50);Cη2 123.8(7.01) |
| S43 | 117.5(9.17) | 176.7 | 61.5(4.39) | 63.3(4.51,4.05) | |
| D44 | 120.6(8.68) | 178.0 | 56.8(4.76) | 41.1(3.01,2.81) | |
| V45 | 107.8(7.15) | 173.8 | 60.4(5.01) | 32.6(2.76) | Cγ 21.5(1.05);Cγ 19.0(1.27) |
| T46 | 109.2(7.40) | 173.8 | 60.5(5.67) | 72.4(4.28) | Cγ 24.8(1.67) |
| P47 | -(-) | 176.7 | 62.3(4.93) | 31.0(2.43,2.07) | Cγ 27.7(2.12,1.99);Cδ 52.1(4.01,3.28) |
| L48 | 117.3(7.24) | 176.6 | 55.3(4.32) | 43.7(1.38,0.59) | Cγ 27.4(1.19);Cδ 26.8(0.57);Cδ 22.6(0.42) |
| N49 | 117.8(8.18) | 172.1 | 52.2(4.74) | 42.8(2.56) | |
| F50 | 118.9(8.37) | 175.6 | 56.6(5.20) | 41.6(2.49,2.06) | Cδ 132.6(6.72);Cε 130.3(6.98); Cζ 128.9(7.17) |
| T51 | 120.2(8.52) | 171.8 | 61.5(4.44) | 71.5(3.71) | Cγ 21.0(1.12) |
| R52 | 128.5(8.52) | 175.3 | 55.3(3.34) | 30.9(1.11,1.58) | Cγ 27.7(0.92,0.87);Cδ 44.2(3.16,3.07) |
| L53 | 127.0(8.98) | - | 53.0(4.68) | 44.2(1.75,1.35) | Cγ 27.1(1.58);Cδ 24.9(0.87) |
| H54 | -(-) | 174.0 | 57.4(4.46) | 31.5(3.28,3.00) | Cδ2 119.3(7.05) |
| D55 | 117.0(7.68) | 174.7 | 52.5(4.62) | 43.9(2.62) | |
| G56 | 106.8(8.32) | 172.8 | 44.5(4.12,3.80) | | |
| I57 | 118.9(8.22) | 175.0 | 60.5(4.16) | 37.4(1.81) | Cγ 27.3(1.52,1.24);Cγm 17.8(0.91); Cδ 11.6(0.87) |
| A58 | 131.5(7.94) | 177.0 | 49.1(4.54) | 22.7(0.95) | |
| D59 | 121.2(8.32) | 177.4 | 58.6(4.41) | 41.2(2.30,2.82) | |
| I60 | 123.9(8.85) | 174.2 | 61.2(4.17) | 39.1(1.84) | Cγ -(1.43,1.33);Cγm 15.2(1.06); Cδ 13.8(0.82) |
| M61 | 127.0(7.48) | 176.7 | 53.8(4.95) | 32.9(2.22,1.86) | Cγ -(2.74);Cε 18.9(2.29) |

| Residue | N (H) | CO | Cα (Hα) | Cβ (Hβ) | Side chain |
|---|---|---|---|---|---|
| I62 | 128.1(9.09) | 174.4 | 60.8(5.42) | 40.7(1.76) | Cγ 28.3(0.79);Cγm 19.0(0.52); Cδ 16.1(0.49) |
| S63 | 117.8(8.82) | 172.4 | 56.8(5.17) | 66.6(3.84) | |
| F64 | 120.7(9.93) | 177.2 | 56.3(5.54) | 41.9(2.94,2.78) | Cδ -(7.07) |
| G65 | 109.5(9.03) | 182.5 | 44.5(4.84,3.60) | | |
| I66 | 116.5(8.43) | 174.4 | 59.7(4.81) | 42.2(1.90) | Cγ 26.7(1.52,1.12);Cγm 18.7(1.00); Cδ 13.5(0.94) |
| K67 | 121.5(9.85) | 177.7 | 57.4(3.85) | 30.3(2.12,2.01) | Cγ 25.4(1.71,1.40);Cδ 28.4(1.83,1.72); Cε 41.9(2.94) |
| E68 | 127.8(8.18) | 174.8 | 57.8(4.31) | 28.5(2.20) | Cγ -(2.45) |
| H69 | -(-) | - | -(-) | -(-) | |
| G70 | -(-) | - | -(-) | | |
| D71 | -(-) | - | -(-) | -(-) | |
| F72 | -(-) | - | -(-) | -(-) | |
| Y73 | -(-) | - | -(-) | -(-) | |
| P74 | -(-) | 178.4 | 63.0(4.37) | 31.6(2.04,1.94) | Cδ 53.9(2.54,2.41) |
| F75 | 118.3(7.97) | 175.9 | 56.9(4.79) | 38.1(3.91,3.09) | Cδ -(7.27) |
| D76 | 116.1(8.35) | 177.4 | 53.4(4.74) | 41.9(3.15,2.67) | |
| G77 | 110.0(8.68) | - | 44.0(4.47) | | |
| P78 | -(-) | - | 63.9(4.05) | 31.7(2.29,1.85) | Cγ 27.7(2.14,2.04) |
| S79 | 124.8(13.02) | 174.4 | 58.4(3.56) | 63.1(4.02,4.24) | |
| G80 | 111.5(8.36) | 173.6 | 46.3(4.02,3.41) | | |
| L81 | 130.1(10.06) | 177.3 | 56.4(3.71) | 41.3(1.77,1.51) | Cγ 27.3(1.38);Cδ 27.3(0.78);Cδ 24.7(0.43) |
| L82 | 127.6(7.98) | 175.5 | 55.9(4.30) | 43.7(1.14,1.07) | Cγ 25.5(1.53);Cδ 25.0(-0.32); Cδ 19.4(-0.54) |
| A83 | 114.3(6.78) | 175.0 | 51.2(4.54) | 22.0(0.87) | |
| H84 | 116.7(8.98) | 171.4 | 54.1(5.14) | 31.3(3.10,2.94) | |
| A85 | 121.2(8.32) | 176.6 | 50.2(5.08) | 23.3(1.45) | |
| F86 | 120.9(8.10) | - | 54.8(4.64) | 41.1(2.76,2.67) | Cδ -(7.17) |
| P87 | -(-) | - | -(-) | -(-) | |
| P88 | -(-) | 174.5 | 64.2(3.11) | 31.7(0.02,0.92) | |
| G89 | 106.9(5.57) | - | 44.2(-) | | |
| P90 | -(-) | - | -(-) | -(-) | |
| N91 | -(-) | - | -(-) | -(-) | |
| Y92 | -(-) | 175.0 | 59.1(4.51) | 36.0(2.42,2.06) | Cδ 138.7(6.90);Cε -(7.18) |
| G93 | 105.4(7.82) | 175.1 | 47.2(3.28,3.86) | | |
| G94 | 119.9(8.02) | 171.7 | 46.8(4.72,4.29) | | |
| D95 | 122.7(8.60) | 173.3 | 56.0(4.61) | 40.2(3.24,3.10) | |
| A96 | 118.4(7.90) | 174.7 | 51.0(4.97) | 22.7(1.24) | |
| H97 | 121.0(9.05) | 173.6 | 50.8(5.93) | 34.7(2.98,2.83) | Cδ2 117.4(7.37) |
| F98 | 122.0(8.82) | 173.9 | 56.9(4.22) | 42.0(2.14,1.99) | Cδ 131.9(6.36);Cε 129.7(6.60); Cζ 127.0(6.46) |
| D99 | 123.0(8.03) | 179.2 | 53.9(3.88) | 41.0(0.98,3.08) | |
| D100 | 129.0(10.20) | 179.5 | 53.4(5.58) | 40.9(2.95,2.63) | |
| D101 | 123.8(9.35) | 177.8 | 56.6(4.98) | 39.1(2.75,2.14) | |

| Residue | N(H) | C' | Cα(Hα) | Cβ(Hβ) | Side chain |
|---|---|---|---|---|---|
| E102 | 114.9(7.34) | 177.5 | 53.1(4.78) | 27.0(1.17,0.52) | Cγ 34.3(1.53,2.61) |
| T103 | 122.1(8.14) | 172.1 | 61.6(4.33) | 68.8(3.94) | Cγ 21.1(1.08) |
| W104 | 132.1(9.59) | 176.3 | 56.1(5.26) | 31.1(3.38,3.00) | Cδ1 128.1(7.49);Nε1 126.0(9.56); Cε3 122.2(7.51);Cζ3 120.8(6.75); Cζ2 115.2(7.86);Cη2 123.1(6.84) |
| T105 | 113.2(8.78) | 174.4 | 60.0(4.96) | 71.4(4.22) | Cγ 19.3(0.79) |
| S106 | 115.7(8.60) | 174.9 | 57.6(4.93) | 63.9(4.14,3.97) | |
| S107 | 121.2(8.97) | 172.8 | 56.9(4.95) | 65.0(4.27,3.91) | |
| S108 | -(-) | 174.8 | 58.0(4.02) | 64.0(3.83,3.49) | |
| K109 | 124.7(7.84) | 175.1 | 55.5(4.30) | 32.1(1.76,1.65) | Cγ 24.9(1.45,1.35);Cδ 28.9(1.78,1.67); Cε 42.1(2.98) |
| G110 | 109.9(7.91) | 173.3 | 44.9(3.79,3.39) | | |
| Y111 | 122.2(8.32) | 173.8 | 58.3(4.05) | 40.4(2.05,1.52) | Cδ 132.4(5.70);Cε 118.4(6.36) |
| N112 | 123.6(8.52) | 175.1 | 54.5(4.96) | 40.9(3.04,2.82) | |
| L113 | 129.8(8.68) | 176.7 | 58.2(4.34) | 41.9(1.61,1.53) | Cγ 26.8(0.88);Cδ 26.8(0.36); Cδ 22.0(-0.18) |
| F114 | 118.5(8.56) | 175.0 | 60.6(4.01) | 37.5(3.44,3.31) | Cδ 132.7(7.31);Cε 130.2(6.83); Cζ 128.7(6.53) |
| L115 | 120.4(8.12) | 178.8 | 57.8(3.19) | 43.4(1.75) | Cγ 27.2(1.74);Cδ 24.9(0.76);Cδ 24.9(0.99) |
| V116 | 115.5(7.80) | 178.6 | 65.9(4.13) | 32.0(2.29) | Cγ 24.1(1.25);Cγ 22.3(1.13) |
| A117 | 122.0(9.34) | 176.8 | 55.3(3.54) | 17.8(1.00) | |
| A118 | 119.0(8.60) | 179.8 | 56.6(3.81) | 17.1(1.05) | |
| H119 | 117.8(7.53) | 176.5 | 58.9(4.60) | 28.7(4.16,3.12) | Cδ2 128.2(7.09) |
| E120 | 118.1(9.19) | 178.1 | 58.8(3.99) | 28.0(2.86,1.85) | Cγ 33.8(1.44,1.04) |
| F121 | 116.9(9.12) | 177.6 | 55.8(4.86) | 36.0(2.81) | Cδ -(6.28);Cε 129.0(6.38);Cζ 127.7(6.10) |
| G122 | 108.9(7.81) | 177.5 | 48.5(4.17,2.51) | | |
| H123 | 121.7(7.32) | 179.5 | 57.6(5.54) | 28.2(2.83,4.12) | Cδ2 -(7.09);Cε1 138.0(6.47) |
| S124 | 117.0(9.00) | 175.4 | 63.1(4.72) | -(4.32) | |
| L125 | 114.7(7.60) | 178.1 | 55.1(4.67) | 43.6(1.75) | Cγ 26.2(2.20);Cδ 24.6(0.53);Cδ 22.2(0.98) |
| G126 | 108.1(8.40) | 172.8 | 45.2(5.06,3.58) | | |
| L127 | 120.7(8.90) | 175.4 | 54.5(4.68) | 41.9(1.57) | Cγ 26.8(1.45);Cδ 26.9(1.05);Cδ 22.3(0.72) |
| D128 | 123.4(8.23) | 174.9 | 50.3(4.04) | 42.5(1.11,2.02) | |
| H129 | 117.0(9.06) | 175.5 | 57.3(5.00) | 29.1(2.87) | Cδ2 125.8(7.19);Cε1 135.7(7.26) |
| S130 | 115.7(6.99) | 175.1 | 56.5(4.21) | 64.3(3.40,4.54) | |
| K131 | 122.3(8.51) | 175.8 | 56.2(4.62) | 32.5(2.09,1.74) | Cγ 25.5(1.51,1.43);Cδ 28.8(1.74); Cε 42.2(3.03) |
| D132 | 124.6(8.86) | 174.2 | 51.3(4.75) | 41.3(2.99,2.47) | |
| P133 | -(-) | 171.8 | 62.6(4.17) | 31.7(2.30,1.55) | Cγ 27.1(1.81,1.68);Cδ 50.7(4.14,3.70) |
| G134 | 106.3(8.52) | 173.4 | 44.5(4.17,3.56) | | |
| A135 | 124.7(8.05) | 177.3 | 52.0(4.61) | 20.0(1.96) | |
| L136 | 132.8(12.17) | 181.3 | 58.0(4.54) | 42.1(1.95,1.63) | Cγ 27.8(1.79);Cδ 22.7(1.28);Cδ 27.4(0.90) |
| M137 | 114.3(9.09) | 177.7 | 53.2(4.63) | 27.2(2.61,2.31) | Cγ 30.6(2.74,3.29);Cε 11.5(0.56) |
| F138 | 128.1(8.06) | 176.9 | 57.3(4.89) | 40.1(3.19,1.99) | Cδ 133.2(7.22);Cε 130.1(6.76); Cζ 128.6(6.92) |
| P139 | -(-) | 172.6 | 63.3(3.65) | 27.6(0.78,0.20) | |

| I140 | 118.8(7.52) | 175.4 | 60.1(4.64) | 40.6(2.00) | Cγ 28.3(1.56,1.24);Cγm 17.5(1.07); Cδ 12.3(0.98) |
|------|-------------|-------|------------|------------|-------------------------------------------------|
| Y141 | 127.4(9.21) | 174.5 | 59.1(4.92) | 38.8(3.30,2.83) | Cδ 133.9(7.13);Cε 118.1(7.04) |
| T142 | 126.2(8.81) | 172.1 | 61.3(4.26) | 70.8(4.03) | Cγ 21.2(1.19) |
| Y143 | 126.0(8.51) | 175.3 | 58.7(4.31) | 39.4(2.94) | Cδ 133.0(7.18);Cε 118.2(6.83) |
| T144 | -(-) | 174.3 | 61.3(4.24) | 69.7(4.21) | Cγ 21.1(1.24) |
| G145 | 110.2(7.24) | 174.2 | 45.8(3.92,3.77) | | |
| K146 | 120.1(7.70) | 176.8 | 56.5(4.32) | 33.0(1.91,1.76) | Cγ 24.8(1.46);Cδ 29.0(1.74);Cε 41.9(3.05) |
| S147 | -(-) | - | -(-) | -(-) | |
| H148 | -(-) | - | -(-) | -(-) | |
| F149 | -(-) | 174.0 | 59.3(4.31) | 40.3(3.16,2.94) | Cδ 132.0(7.25);Cε 131.0(7.22) |
| M150 | 126.9(7.25) | 173.8 | 53.4(4.37) | 34.7(1.85,1.69) | Cγ 31.5(2.37) |
| L151 | 127.2(8.40) | 174.2 | 53.3(4.14) | 42.9(1.66,1.34) | Cγ 25.0(0.42);Cδ 25.8(0.82);Cδ 25.8(0.48) |
| P152 | -(-) | 176.2 | 62.9(4.36) | 33.2(2.32,1.93) | Cγ 28.7(-);Cδ 51.0(-) |
| D153 | 120.7(8.40) | 178.0 | 58.0(4.33) | 41.2(2.69) | |
| D154 | 116.8(8.90) | 177.3 | 58.8(4.43) | 43.8(3.04,2.37) | |
| D155 | 114.5(7.15) | 178.6 | 56.5(4.81) | 43.6(2.79,2.92) | |
| V156 | 119.3(7.95) | 178.1 | 67.0(3.58) | 31.8(2.30) | Cγ 23.3(1.10);Cγ 21.3(0.95) |
| Q157 | 117.1(8.72) | 179.9 | 58.6(3.90) | 28.1(2.20) | Cγ 34.3(2.70,2.52) |
| G158 | 108.5(8.28) | 176.3 | 46.6(2.92,1.93) | | |
| I159 | 125.3(9.02) | 178.4 | 61.2(4.42) | 38.7(2.35) | Cγ 30.6(2.07,1.83);Cγm 21.1(1.63); Cδ 15.4(1.04) |
| Q160 | 122.4(8.57) | 179.4 | 58.4(4.23) | 26.9(1.78,2.18) | Cγ 34.6(-) |
| S161 | 119.7(7.95) | 175.0 | 61.8(4.27) | 61.1(-) | |
| L162 | 120.9(6.78) | 177.7 | 56.5(4.21) | 44.6(1.84,0.39) | Cγ 25.3(1.60);Cδ 23.2(0.80);Cδ 25.9(1.00) |
| Y163 | 114.0(7.65) | 175.8 | 58.9(4.79) | 41.2(3.49,2.76) | Cδ 134.2(7.39);Cε 117.9(7.42) |
| G164 | 109.5(8.35) | 180.3 | 44.5(4.34,4.08) | | |

Footnotes to Table S1

[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, $^{13}$C and $^{15}$N chemical shifts are referenced according to the method of Wishart et al. 1995