### B

| Residue | N     | NH | αH | βH     | Others                                      |
|---------|-------|----|----|--------|---------------------------------------------|
| D1      | 117.07| 8.88| 4.38| 2.49, 2.84 | 5.08                                        |
|         | 118.01| 8.66| 4.61| 2.53, 2.72 | 5.03, 5.23                                   |
| X2      |       |    | 3.67| 2.06   | γCH₂: 1.48, 2.20; δCH₂: 3.47, 3.84; ε: 1.21, 1.49 |
|         |       |    | 3.70| 2.04   | γCH₂: 1.50, 2.19; δCH₂: 3.47, 3.84; ε: 1.21, 1.49 |
| V3      | 116.15| 7.72| 4.25| 1.81   | Hγ1# 0.76; Hγ2# 0.91                         |
|         | 116.24| 7.75| 4.25| 1.82   | Hγ1# 0.76; Hγ2# 0.76                         |
| D4      | 120.64| 8.62| 4.72| 2.50, 2.65 |                                             |
| V5      | 107.15| 8.69| 4.51| 2.13   | Hγ1# 0.93; Hγ2# 0.93                         |

**Supplementary Figure S1. Bosc et al., 2021**