**Table S1.** 1H Chemical Shifts (ppm) for Anal 3-Pro in SDS Micelles at 318K, pH 4.0

| Residue | Chemical shift (ppm)a | 3*J*HNαH |
| --- | --- | --- |
| NH | αH | βH | Others |
| Ala 2 |  |  |  |  |  |
| Lys 3 |  |  |  |  |  |
| Lys4 | 8.11 | 4.20 | 1.81 | rCH2 1.44 | 3 |
| Val5 | 7.83 | 3.86 | 2.03 | rCH3 0.82,0.64 | 4 |
| Phe6 | 7.67 | 4.42 | 3.22, 3.11 | 2,6H 7.32 |  |
| Lys7 | 7.83 | 4.16 | 1.90 | rCH2 1.48 |  |
| Arg8 | 7.9 | 4.14 | 1.90 | rCH2 1.75 |  |
| Leu9 | 7.67 | 4.19 | 1.88 | rH1.45 /δCH3 0.94,0.82 |  |
| Pro10 |  | 3.72 | 2.35 , 2.19 | rCH21.83 / δCH23.63 |  |
| Lys11 | 8.27 | 4.28 | 1.93 , 1.74 | rCH2 1.51/ εCH23.14 | 48 |
| Leu12 | 7.79 | 4.10 | 1.63 | rH 1.31 /δCH3 0.89,0.81 | 36 |
| Phe13 | 8.38 | 4.28 | 3.14 | 2,6H 7.13 |  |
| Ser14 | 8.17 | 4.26 | 4.09 |  | 10 |
| Lys15 | 7.79 | 4.21 | 2.06 , 1.69 | rCH2 1.55 | 5 |
| Ile16 | 7.93 | 3.89 | 1.97 | rCH3 0.96 | 5 |
| Trp17 | 8.52 | 4.34 | 3.31 , 3.19 | 4H 7.47 / 2,6H 7.17 / 5H 6.96 |  |
| Asn18 | 8.05 | 4.49 | 2.86 | rNH2 6.91 |  |
| Trp 19 | 7.97 | 4.49 | 3.48 , 3.39 | 4H7.56 / 2,6H 7.27 |  |
| Lys20 | 7.97 | 3.75 | 1.64 | rCH21.16 / εNH36.90 | 5 |

*a*Chemical shifts are relative to DSS (0 ppm)