|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **SPN10** | **H** | **N** | **Ha** | **Ca** | **Hb** | **Cb** | **other** |
| Trp1 | - | - | 4.16 | 57.02 | 3.13 | 30.24 | H 7.06; H 9.99; H 7.44; H 7.39; H 7.01; H 7.13; C 128.61; C 121.21; C 115.27;  C 122.73; C 125.34; N 130.32 |
| Arg2 | 8.15 | 123.39 | 4.14 | 56.79 | 1.48, 1.54 | 32.00 | H 1.32; H 2.99; Hsc 6.90, 7.05; C 27.47;  C 43.86, N 96.86 |
| Trp3 | 8.01 | 123.13 | 4.43 | 57.62 | 3.12 | 30.16 | H 7.16; H 10.09; H 7.56; H 7.33; H 7.08; H 7.16; C 127.99; C 121.52; C 115.34;  C 122.75; C 125.37; N 129.51 |
| Lys4 | 7.96 | 124.35 | 4.00 | 56.80 | 1.48, 1.59 | 33.68 | H 1.14, H 1.48; H 2.78; C 25.01; C 29.87;  C 42.61 |
| C’NH2 | 6.67, 6.77 | 107.45 |  |  |  |  |  |
| **SS-20** | **H** | **N** | **Ha** | **Ca** | **Hb** | **Cb** | **other** |
| Phe1 | - | - | 4.11 | 57.45 | 3.05, 3.24 | 40.36 | H 7.25; H 7.33; H 7.29; C 132.00; C 130.59; C 130.07 |
| *arg2* | 7.06 | N.D. | 4.15 | 56.16 | 1.16, 1.20 | 30.63 | H 0.72, 0.76; H 2.83; Hsc 6.90, 7.13;C 26.61;  C 43.11; N 96.80 |
| Phe3 | 8.75 | 122.21 | 4.74 | 57.51 | 2.92, 3.28 | 39.80 | H 7.33; H 7.36; H 7.42; C 131.90; C 131.62; C 131.83 |
| Lys4 | 8.45 | 123.48 | 4.30 | 56.17 | 1.79, 1.87 | 33.08 | H 1.43, 1.48; H1.67,1.71; H 2.99; C 24.92;  C 29.10; C 41.88 |
| C’NH2 | 7.22, 7.43 | 108.63 |  |  |  |  |  |
| **SPN4** | **H** | **N** | **Ha** | **Ca** | **Hb** | **Cb** | **other** |
| *arg1* | - | - | 3.96 | 54.35 | 1.66 | 29.84 | H 1.11, 1.12; H 3.01; C 24.19; C 41.79 |
| Tyr2 | 8.86 | 118.64 | 4.73 | N.D. | 2.76, 3.08 | 37.87 | H 7.18; H 6.87; C 131.97; C 117.02 |
| Lys3 | 8.52 | 123.10 | 4.33 | 55.02 | 1.74, 1.67 | 31.94 | H 1.40, 1.34; H 1.66; H 3.00; C 23.21; C 27.85; C 40.85 |
| Phe 4 | 8.30 | 122.15 | 4.65 | 55.75 | 3.08, 3.21 | 38.37 | H 7.36; H 7.38; H 7.30; C 130.74; C 130.22; C 128.83 |
| C’NH2 | 7.16, 7.65 | 109.26 |  |  |  |  |  |
| **SS-31** | **H** | **N** | **Ha** | **Ca** | **Hb** | **Cb** | **other** |
| *arg1* | - | - | 3.89 | 55.34 | 1.69 | 31.21 | H 1.29; H 3.13; C 25.55; C 43.09 |
| Tyx2 | 8.81 | 122.40 | 4.75 | 61.92 | 2.96, 3.17 | 33.17 | H 2.24; H 6.56; C 21.72; C 117.28 |
| Lys3 | 8.08 | 124.01 | 4.32 | 56.00 | 1.71, 1.66 | 33.12 | H 1.27, 1.33; H 1.65; H 2.97; C 23.96; C 28.82; C 41.78 |
| Phe4 | 8.36 | 122.16 | 4.58 | 57.10 | 3.07, 3.17 | 39.24 | H 7.41; H 7.35; H 7.31; C 131.16; C 131.48; C 129.59 |
| C’NH2 | 7.16, 7.65 | 109.26 |  |  |  |  |  |

*a*NMR data were collected on 10 mM peptide samples, at pH 6, and a temperature of 25°C. The samples contained no added buffers or salts. Chemical shifts were referenced using 3-(Trimethylsilyl)propane-1-sulfonate (DSS) and are given in units of ppm. Because the free and bicelle-bound peptides are in fast exchange, and since there is an excess of the peptides, the chemical shift assignments in this table are also valid for the bound peptides.

*b*Underlined 1H chemical shifts show significant differences of ~0.4 ppm from the random coil values reported in Table 2.3 of Wüthrich, K. NMR of Proteins and Nucleic Acids. (John Wiley & Sons, New York; 1986). These upfield shifts are characteristic of aromatic ring current effects, and likely reflect basic residues involved in cation-pi interactions with aromatic rings.