

Supplementary Table II – Hydrophobicity, pI and average charge of peptides at pH

7.4. The free energy of transfer from aqueous to apolar media was calculated according to the scale proposed by WIMLEY; WHITE (1996). Average charge in physiological pH and pI was calculated using the ideal model as described in TEIXEIRA; LUND; DA SILVA (2010).

| Peptide | $\Delta G_{\text{Hydrophobicity}}$ (kcal/mol) | pI | Average charge in pH 7,4 |
|----------------|---|-----------|-------------------------------------|
| TS 1a | 1.71 | 4.0 | -1.44 |
| TS 1b | -0.45 | 5.5 | -0.44 |
| TS 2 | 0.23 | 10.0 | 1.56 |
| TS 3 | 1.67 | 4.4 | -1.45 |
| TS 4 | 1.68 | 11.0 | 2.55 |
| TS 5 | -1.82 | 5.8 | -0.45 |
| TS 6 | -1.20 | 5.1 | -1.37 |
| TS 7 | 3.57 | 4.5 | -1.44 |
| TS 8 | -0.09 | 5.2 | -0.44 |
| TS 9 | -1.28 | 5.5 | -0.44 |
| TS 10 | 2.12 | 6.0 | -0.45 |
| FLY | -0.18 | 8.7 | 0.55 |

TEIXEIRA, A. A. R.; LUND, M.; DA SILVA, F. L. B. Fast Proton Titration Scheme for Multiscale Modeling of Protein Solutions. **J. Chem. Theory Comput.**, v. 6, n. 10, p. 3259–3266, 2010.

WIMLEY, W. C.; WHITE, S. H. Experimentally determined hydrophobicity scale for proteins at membrane interfaces. **Nature structural biology**, v. 3, n. 10, p. 842–848, out. 1996.