Membrane Adsorption Enhances Translocation of Antimicrobial Peptide Buforin 2

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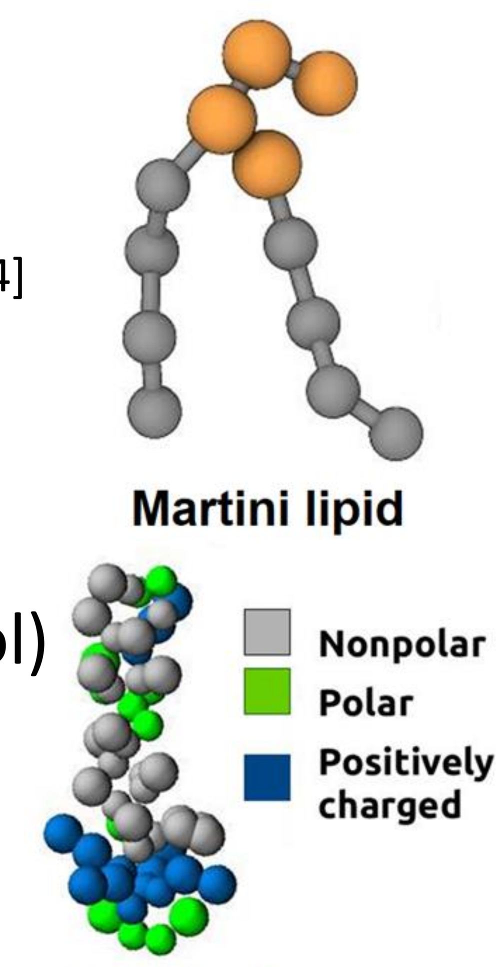
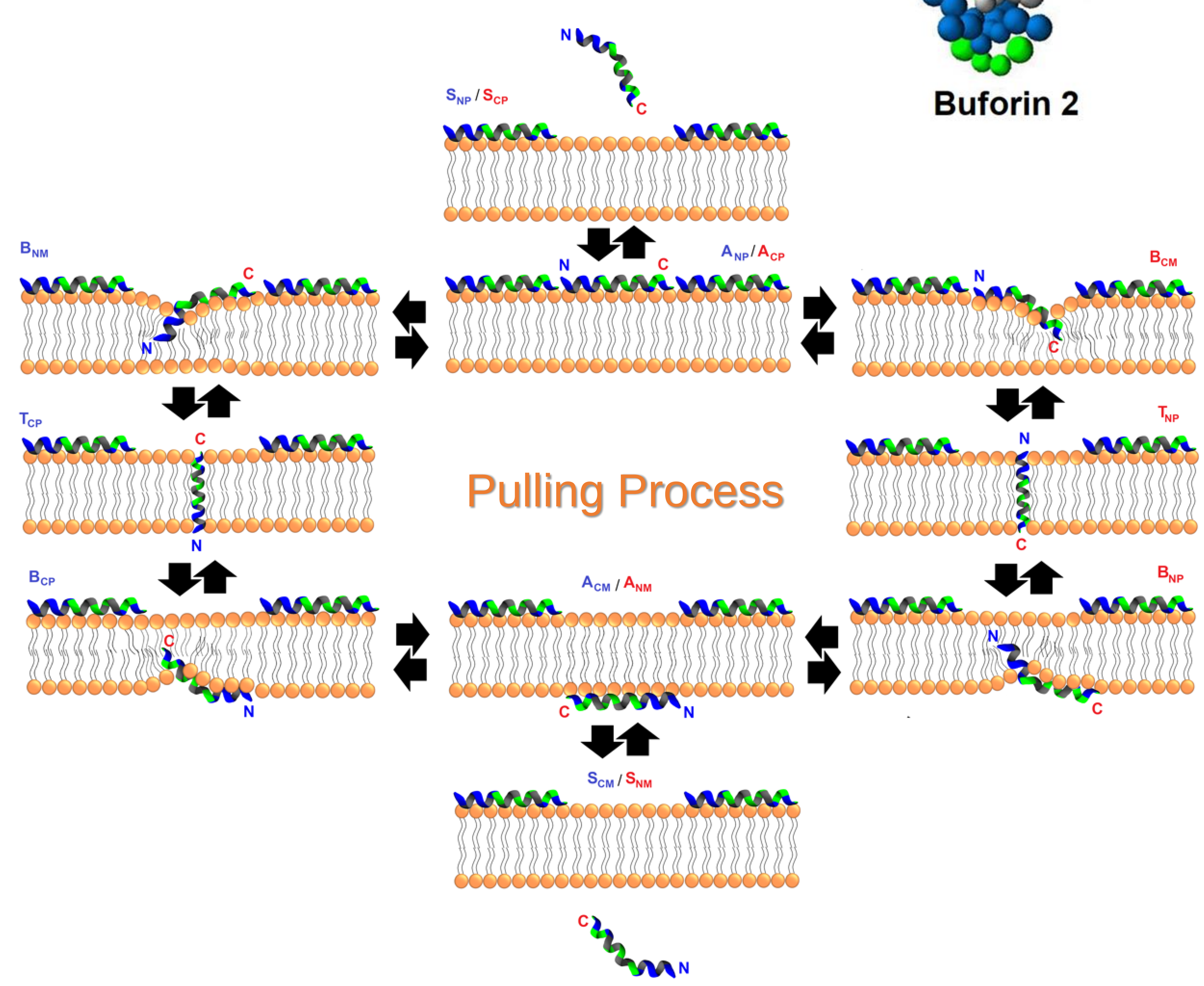
MOTIVATION

- **Buforin 2 is a promising antimicrobial peptide (AMP) alternative to antibiotics.** [1]
- **Buforin 2 can readily enter bacterial cells and kill them in a non-lytic manner.** [2]
- **Asymmetry is a suggested critical factor contributing to AMPs' translocation across cell membranes.** [3]

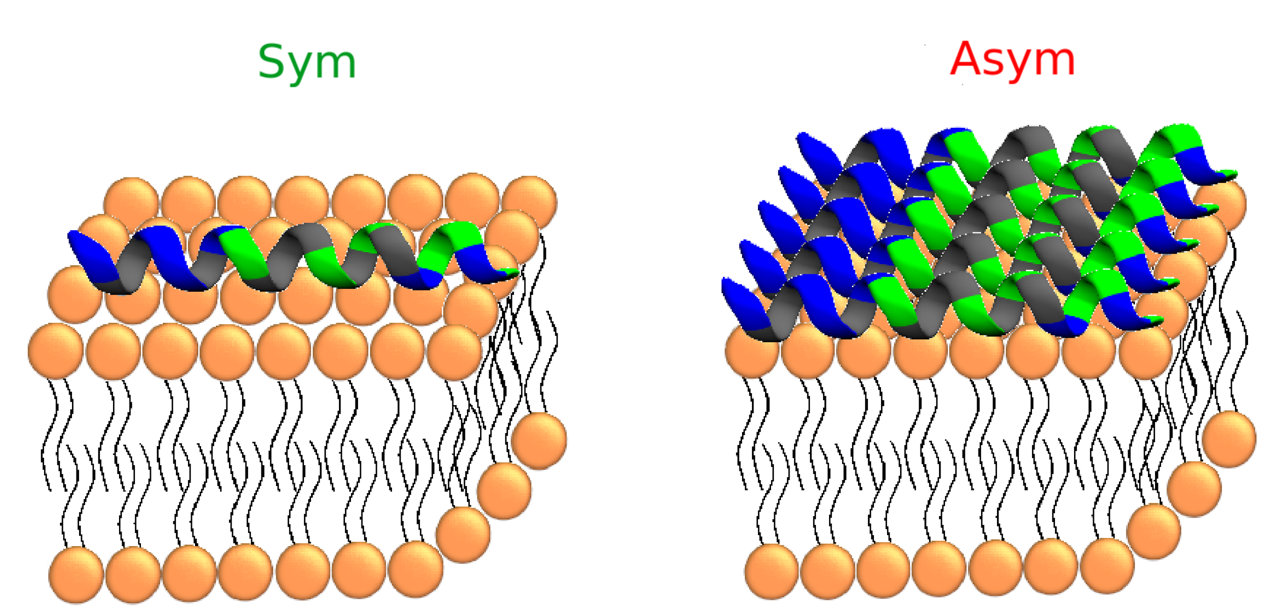
METHODS

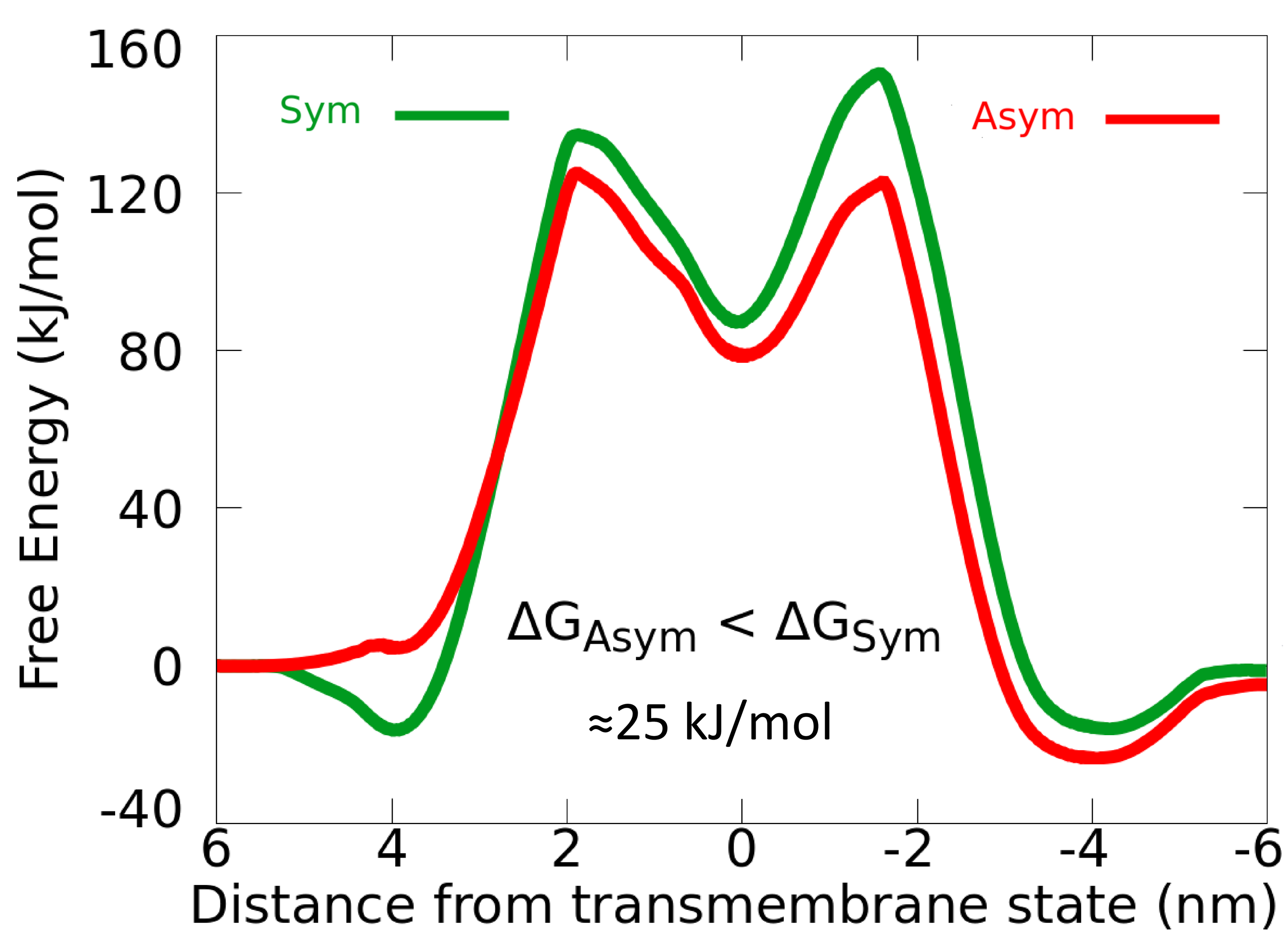
- **Molecular Dynamics Simulations:**
  GROMACS program package v 2020.3 [4]
  Coarse-grained Martini 3 Force Field [5]
- **NPT Ensemble at 310 K and 1 bar**
- **MEMBRANE:** POPE:POPG (3:1 mol:mol)
- **AMP:** Buforin 2 (21 residues)

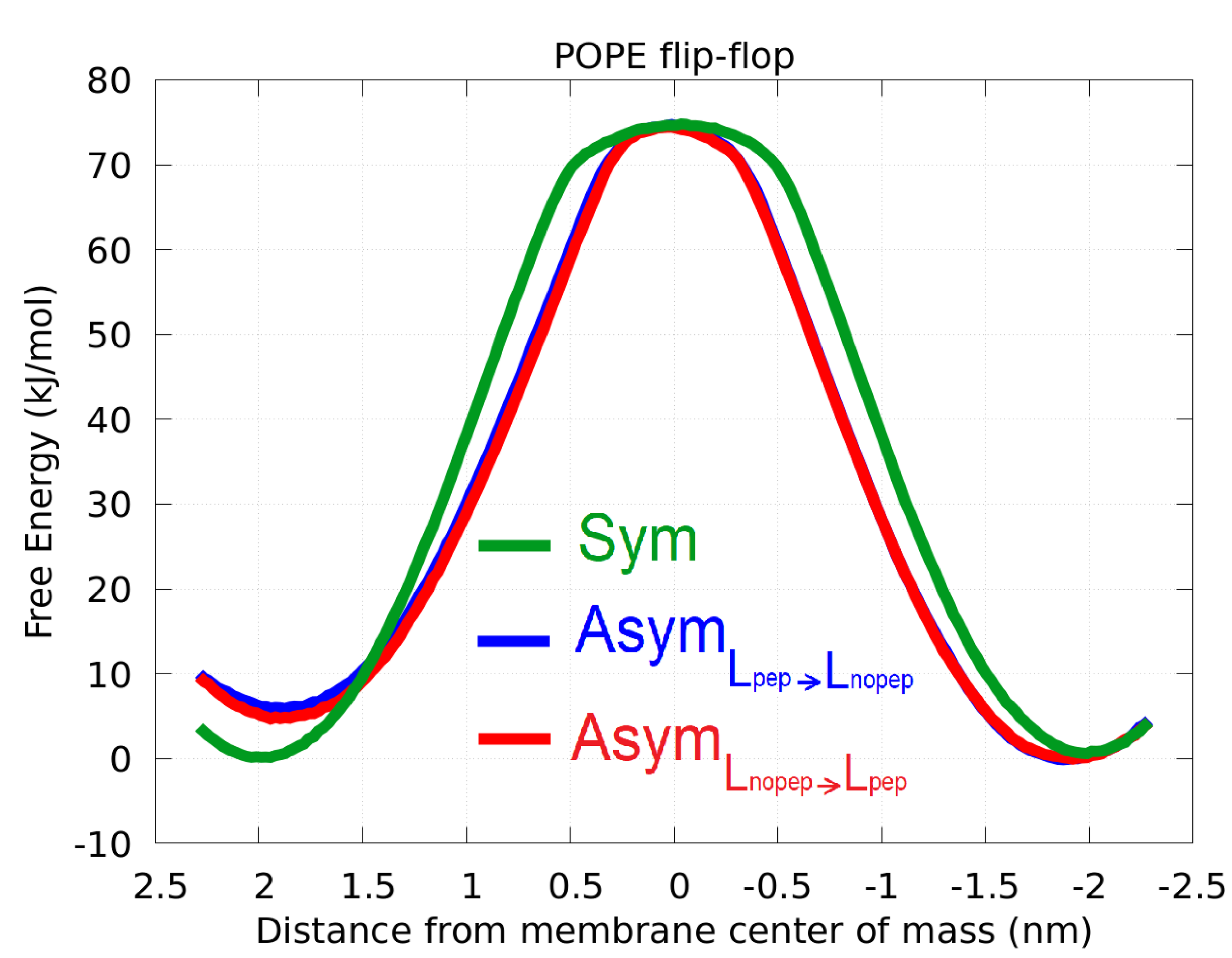


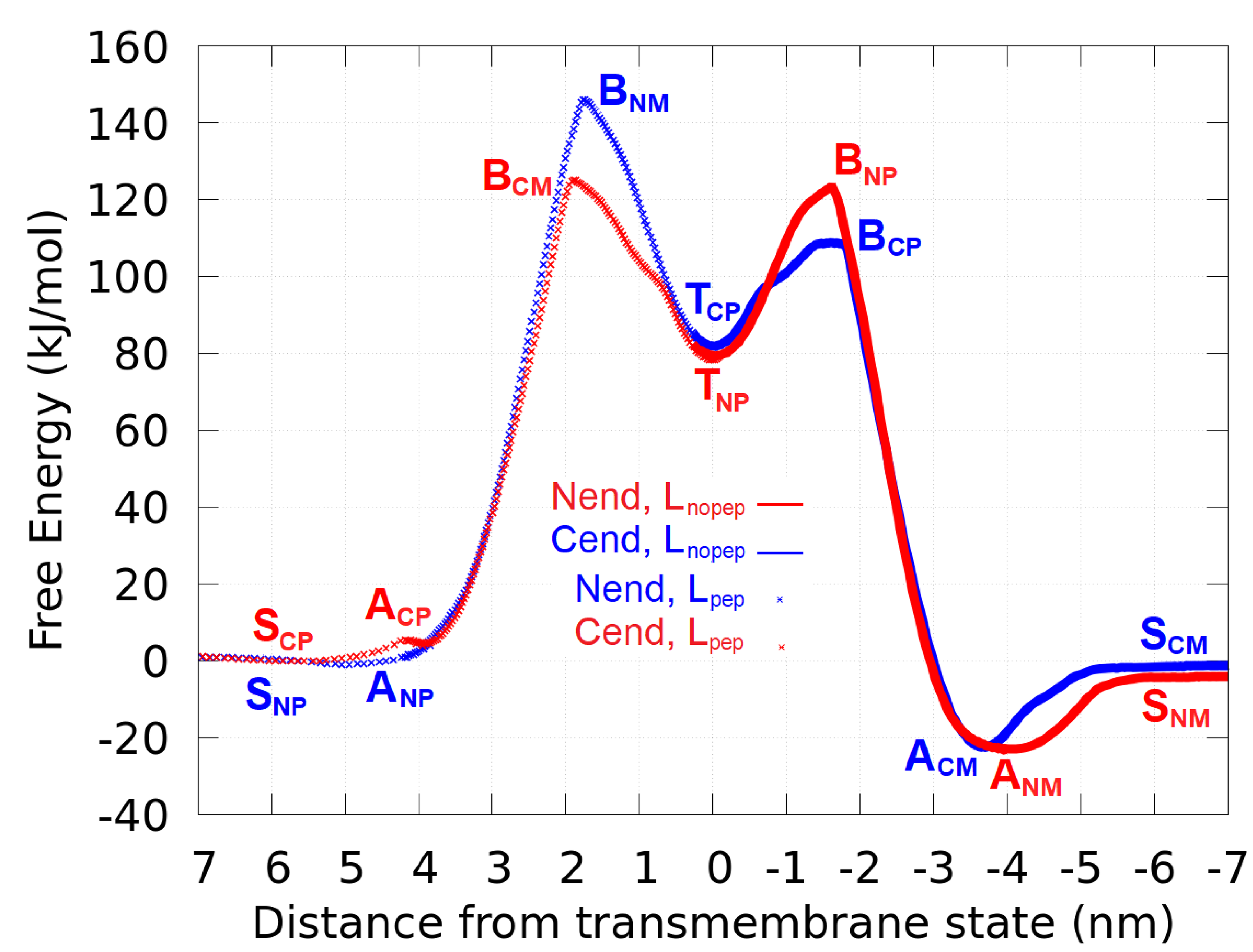


RESULTS









CONCLUSIONS

Membrane adsorption on one of the leaflets:

- ✓ **plays an important role in membrane transport.**
- ✓ **significantly enhances the translocation of AMPs.**
- ✓ **perturbs the lipid packing and facilitates lipid flip-flop.**

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3) Scott H., et al.: *Biophys. J.* 2019, 116 (8) 1495—1506.
4) Abraham M., et al.: *SoftwareX* 2015, 1-2, 19—25.
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Financováno Evropskou unií NextGenerationEU

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