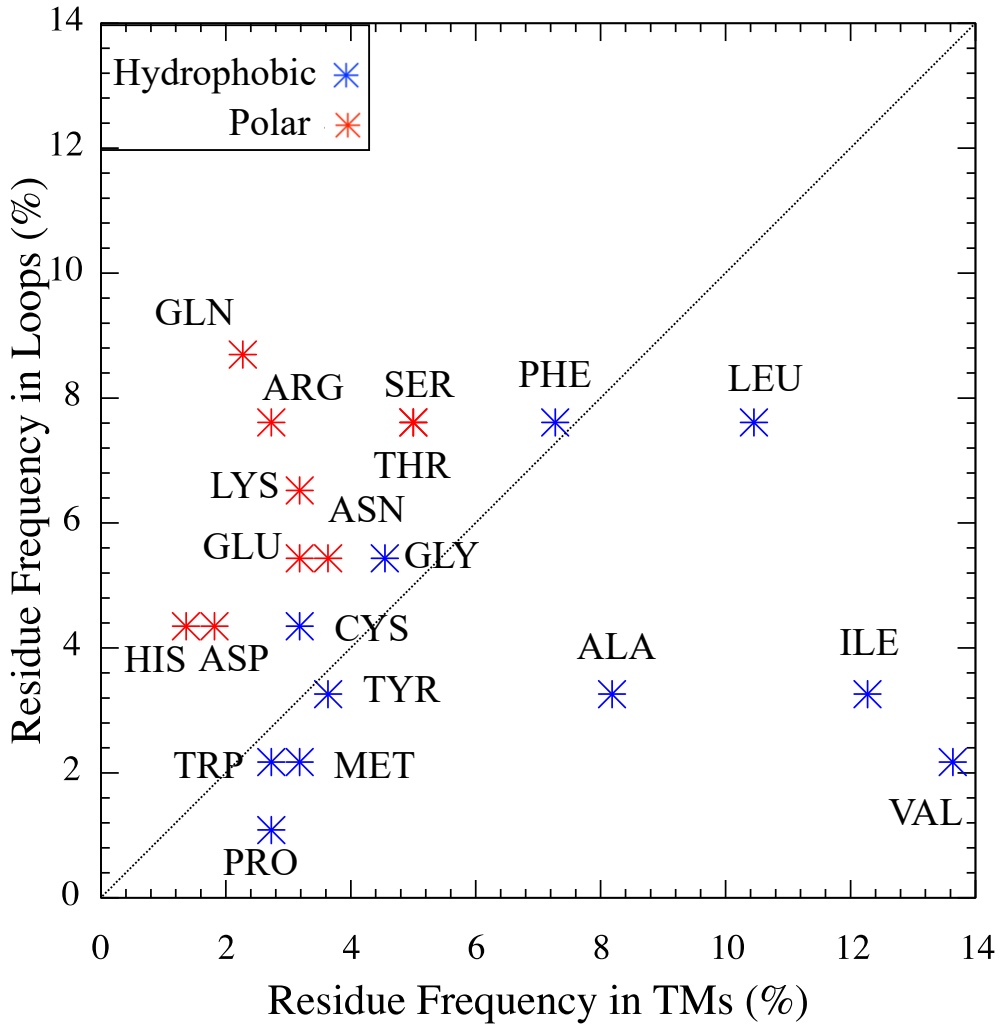
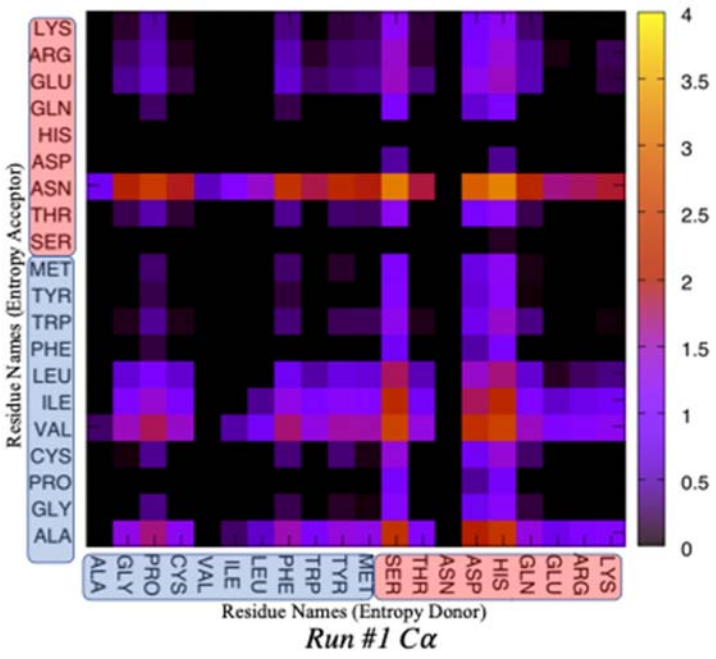
SUPPLEMENTARY MATERIALS:

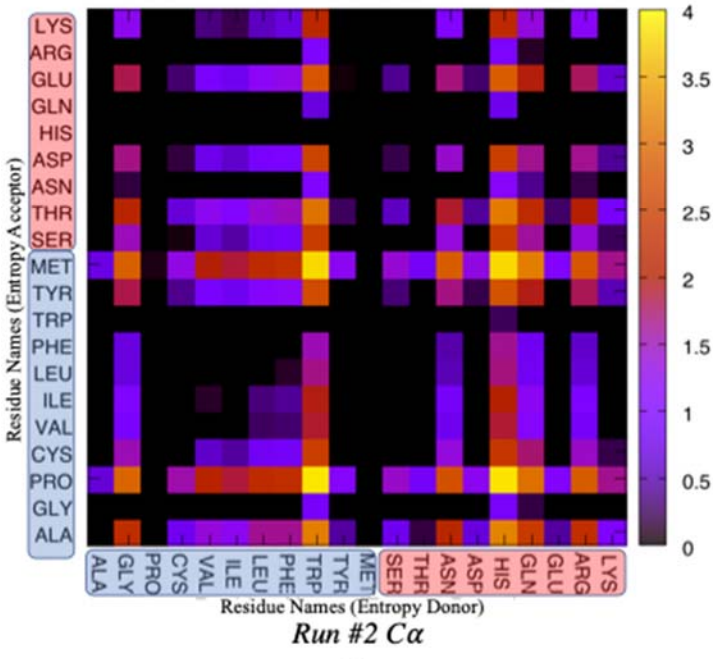


Supplementary Figure S1. Residue frequency (%) of each residue type in loop and transmembrane (TM) regions.



Run #1 Cα

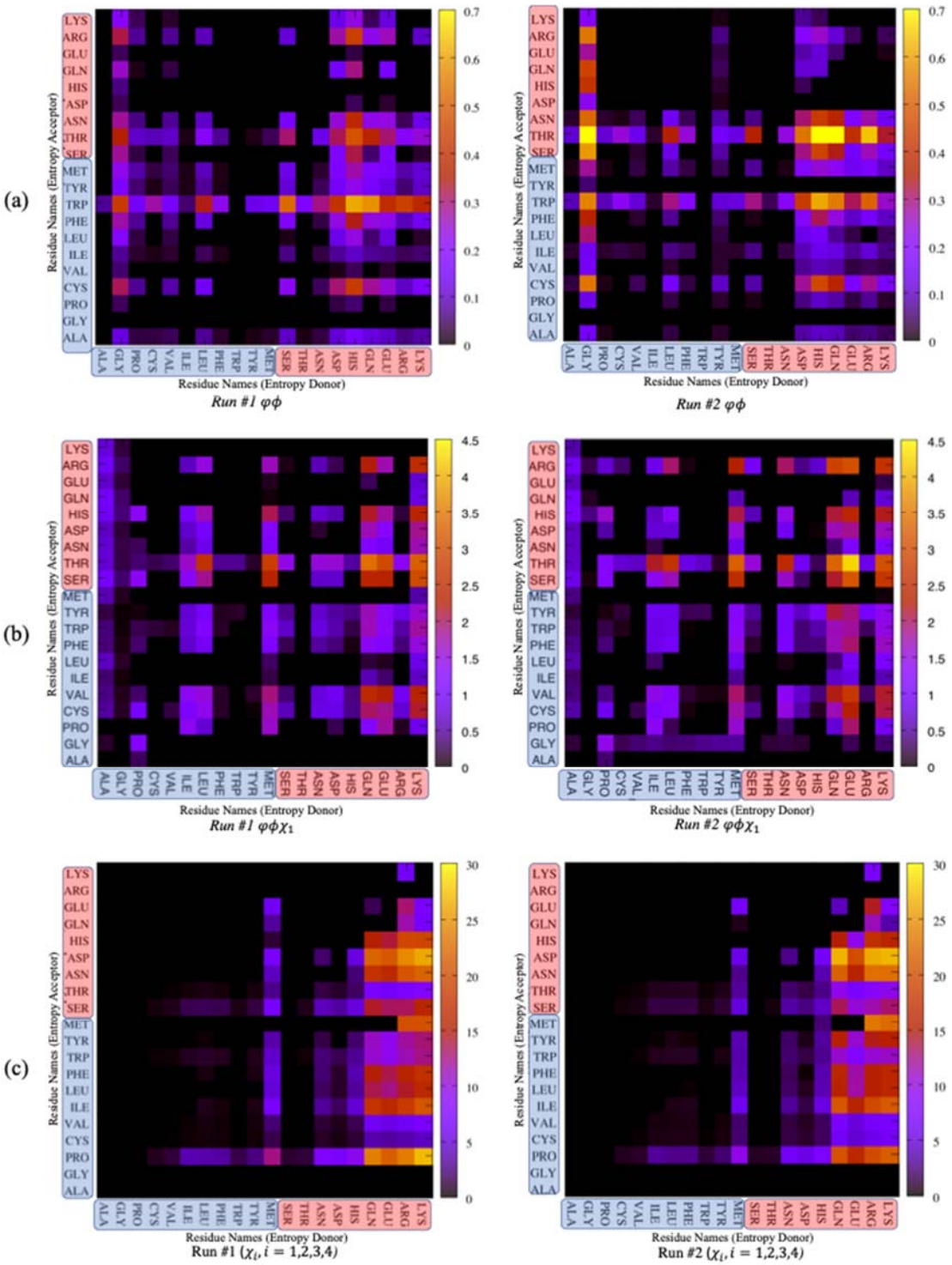
(a)



Run #2 Cα

(b)

Supplementary Figure S2. (a),(b) Average net transfer entropy based on Cα fluctuations for residue pairs classified as either hydrophobic (blue) or polar (pink) for two MD runs



Supplementary Figure S3. (a),(b) Average net transfer entropy for residue pairs classified as either hydrophobic (blue) or polar (pink) for two MD runs based on rotameric states of (a) backbone torsion angles, (ϕ, ψ), (b) backbone torsion angles, (ϕ, ψ) and the first side-chain torsion angle (χ_1) and (c) all possible side-chain torsion angles $\chi_k, k = 1,2,3,4$.