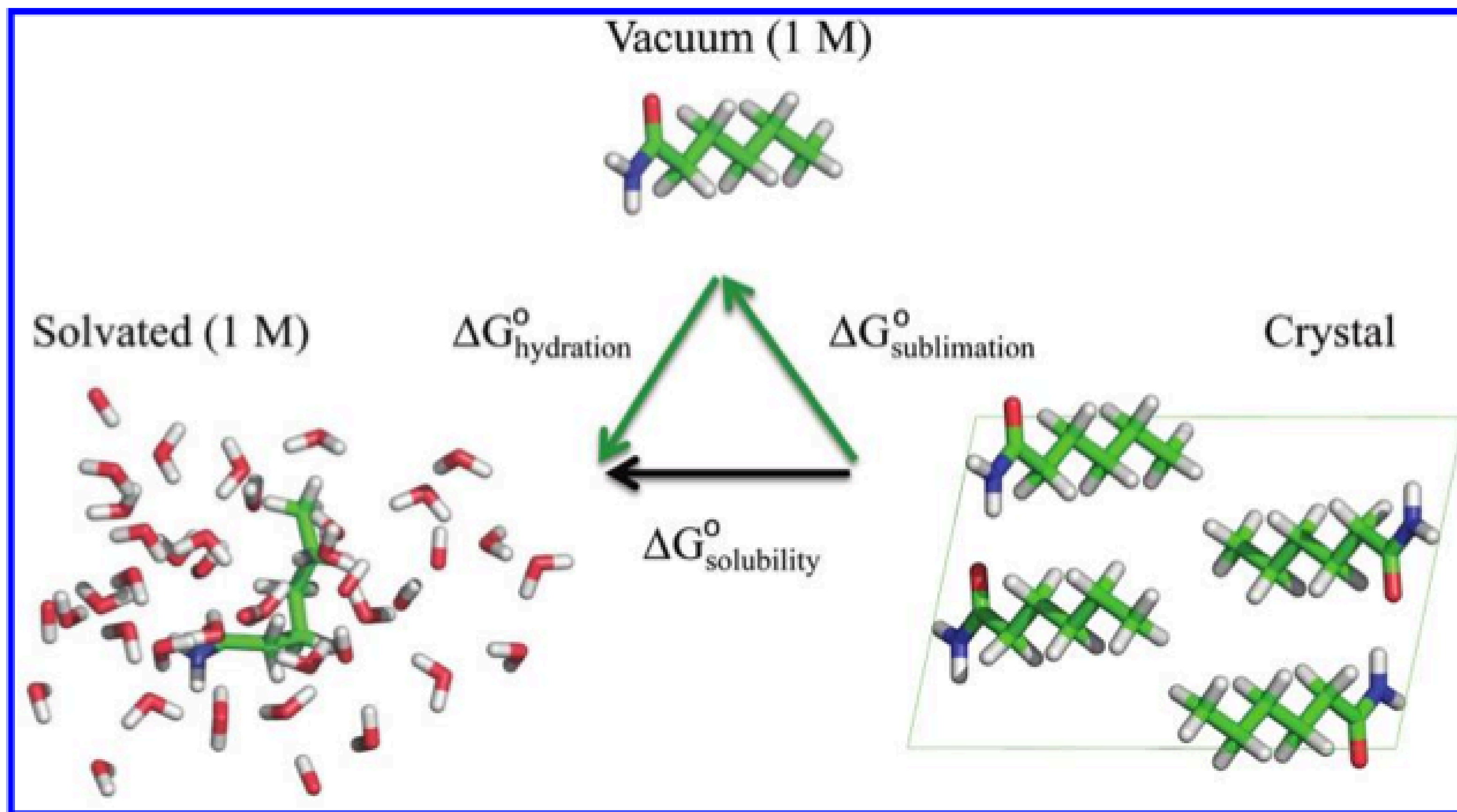
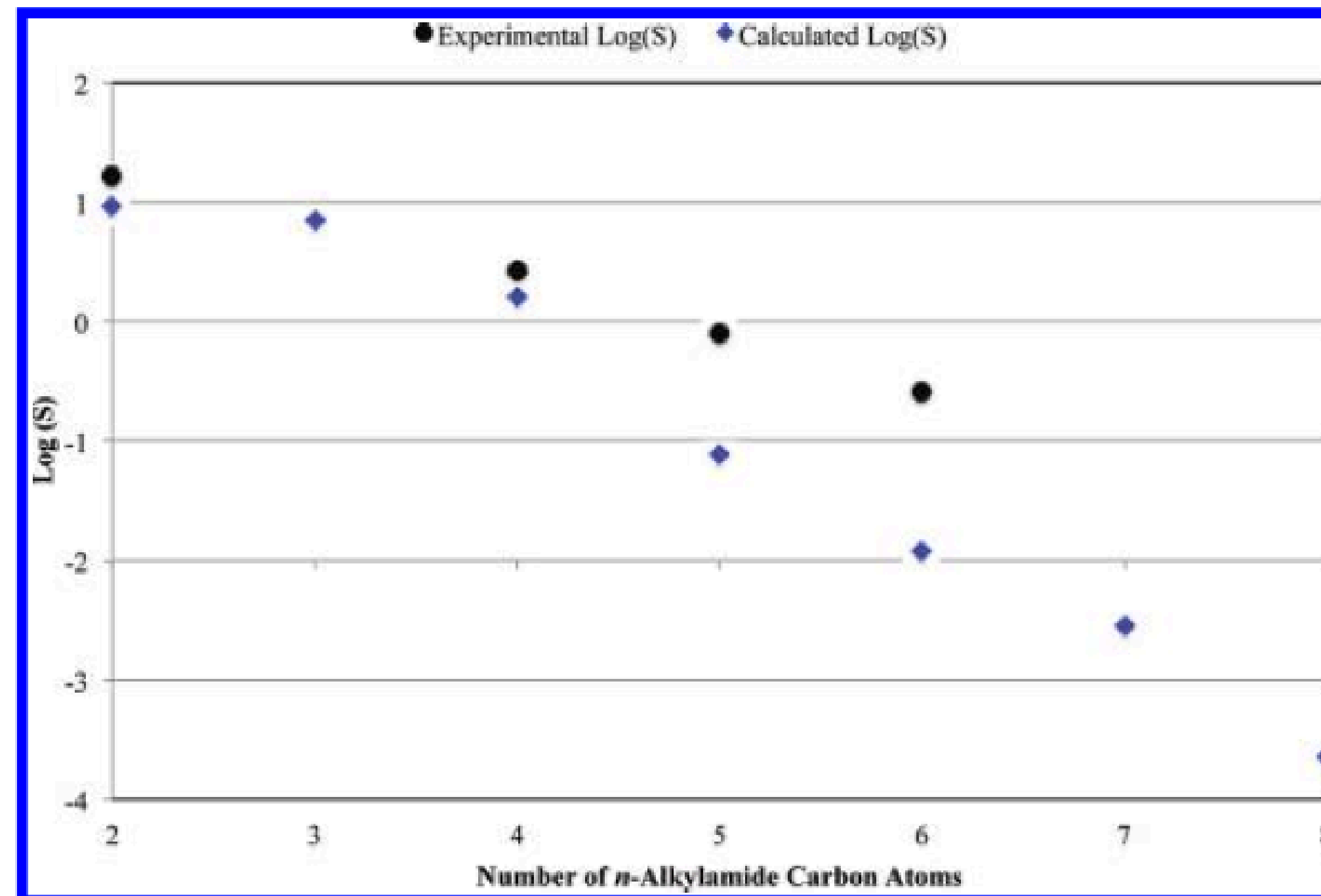


# A thermodynamic cycle for solubility



From Ref [8]. Note that solubility  $\neq$  solvation or hydration.  
Hydration + sublimation free energies calculated with alchemical free energy methods.

# Results on an initial series appear promising without any tuning



**Figure 5.** Shown are experimental and calculated  $\log(S)$  values for the *n*-alkylamides (*S* has units of mol/L) from acetamide to octanamide. There is a monotonic trend in both the experimental and calculated values toward lower solubility with each additional  $\text{CH}_2$  group due to increasingly favorable deposition and to a lesser extent from unfavorable solvation.

From Ref [8]