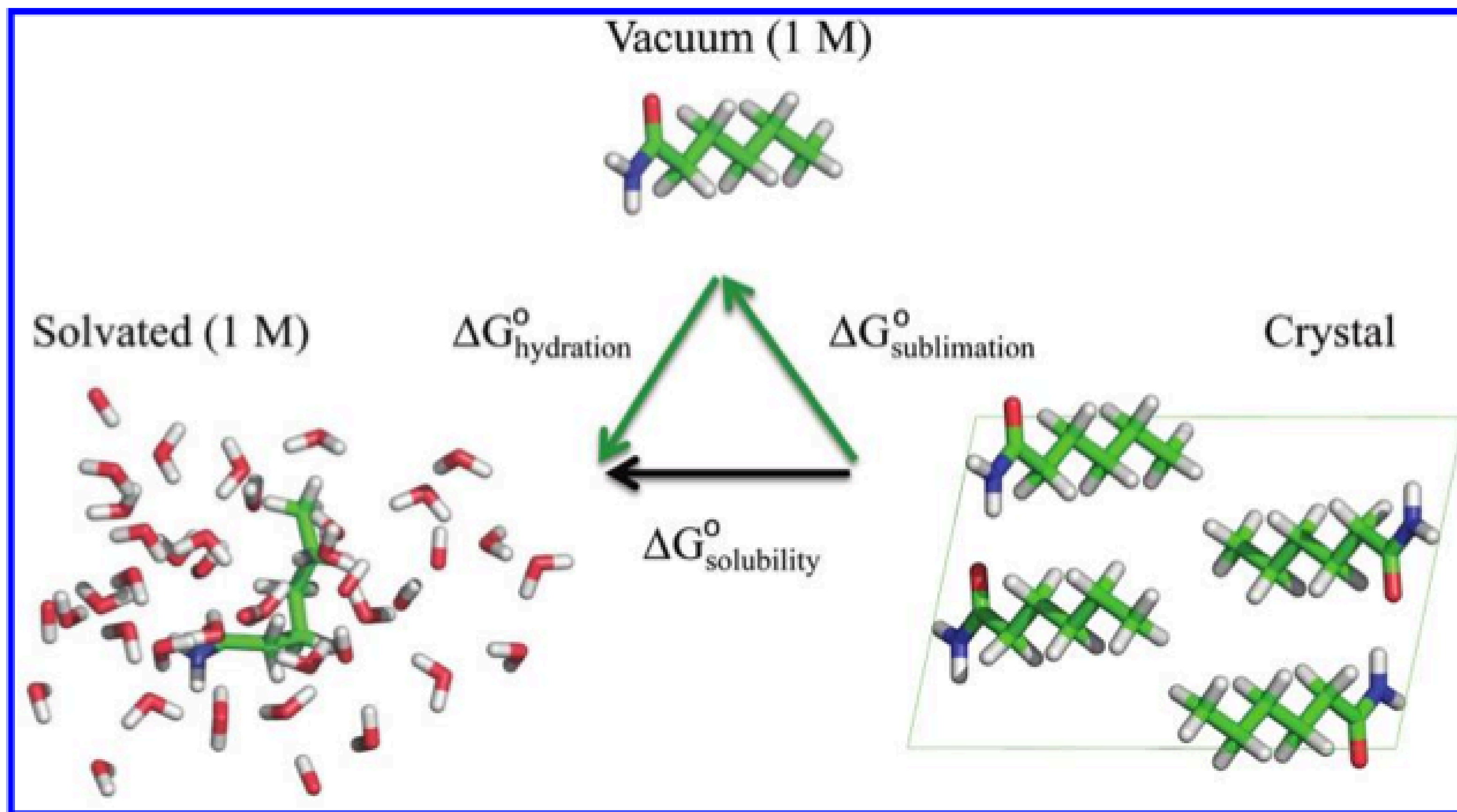


A thermodynamic cycle for solubility



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

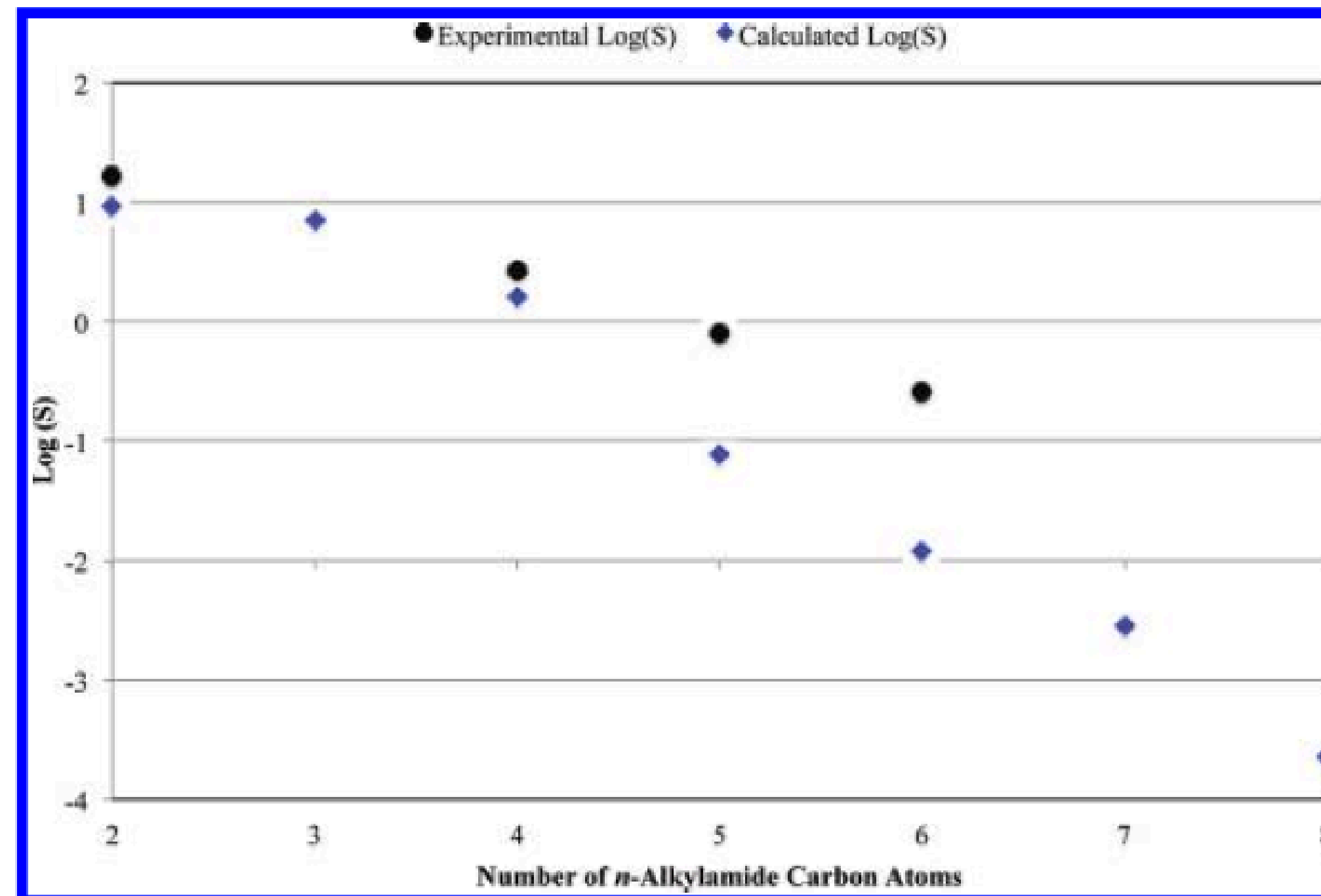


Figure 5. Shown are experimental and calculated $\log(S)$ values for the n -alkylamides (S has units of mol/L) from acetamide to octanamide. There is a monotonic trend in both the experimental and calculated values toward lower solubility with each additional CH_2 group due to increasingly favorable deposition and to a lesser extent from unfavorable solvation.

From Ref [8]