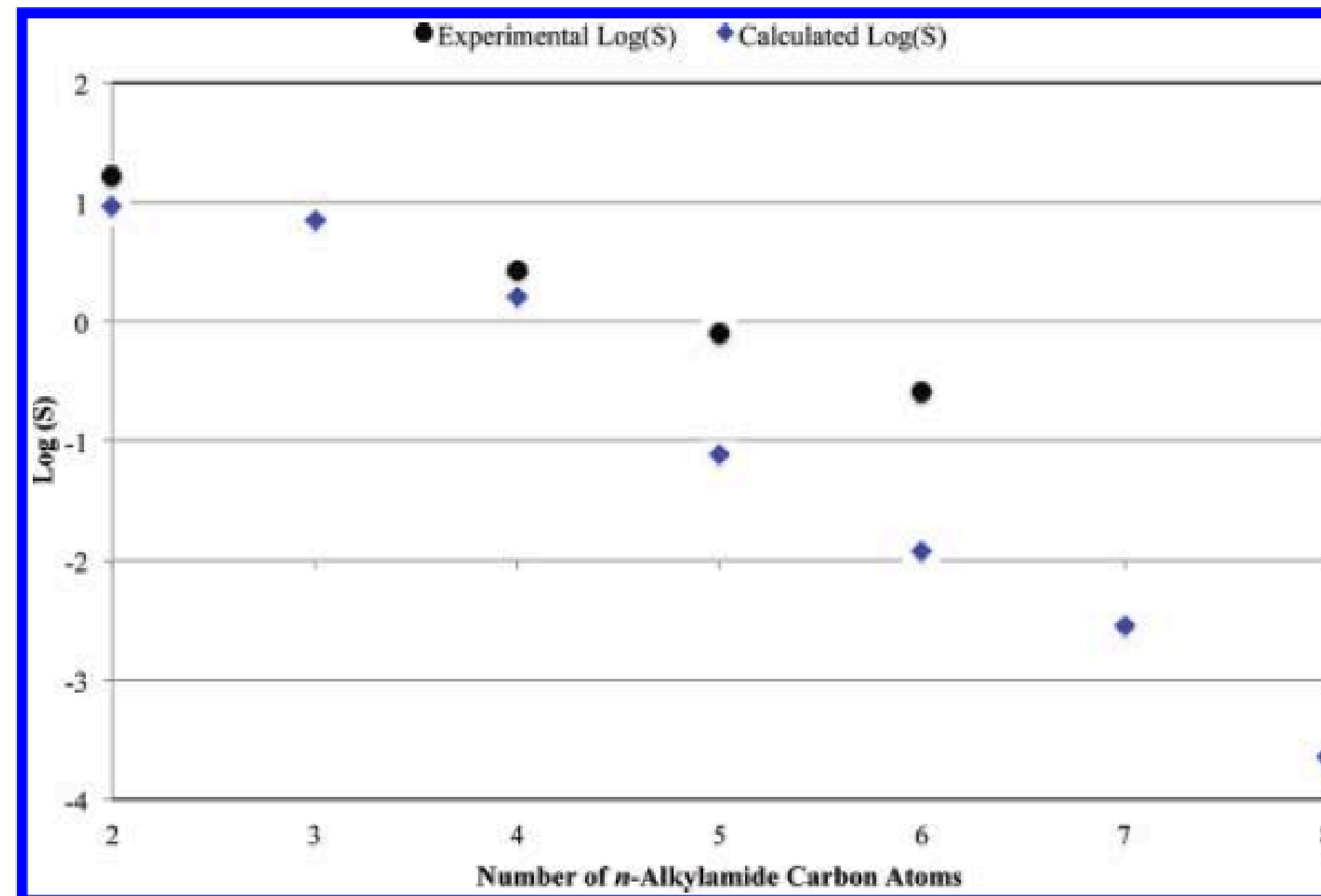


# Results on an initial series appear promising without any tuning



**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]

# References

- [1] Many parts of today's lecture were adapted from a lecture by David Mobley ([https://github.com/MobleyLab/drug-computing/tree/master/uci-pharmsci/lectures/free\\_energy\\_basics](https://github.com/MobleyLab/drug-computing/tree/master/uci-pharmsci/lectures/free_energy_basics)) under the CC BY 4.0 license. The lecture is part of the Drug Discovery Computing Techniques course (PharmSci 175/275) at UC Irvine.
- [2] Llinàs, A.; Glen, R. C.; Goodman, J. M. Solubility Challenge: Can You Predict Solubilities of 32 Molecules Using a Database of 100 Reliable Measurements? J. Chem. Inf. Model. 2008, 48 (7), 1289–1303. <https://doi.org/10.1021/ci800058v>.
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