Results on an initial series appear promising without any tuning

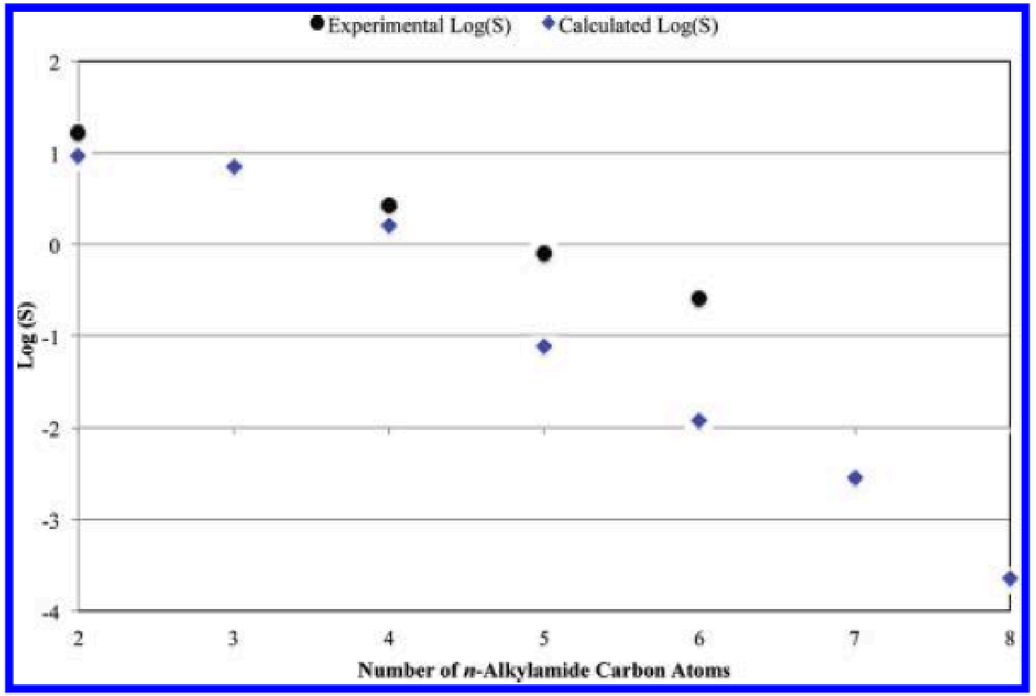

Figure 5. Shown are experimental and calculated log(*S*) values for the *n*-alkylamides (*S* has units of mol/L) from acetamide to octanamide. There is a monotonic trend in both the experimental and calculated values toward lower solubility with each additional CH_2 group due to increasingly favorable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

From Ref [8]

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) under the CC BY 4.0 license. The lecture is part of the Drug Discovery Computing Techniques course (PharmSci 175/275) at UC Irvine.
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