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Erratum

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Correction to Small Molecule Hydration Free Energies in Explicit Solvent: An Extensive Test of Fixed-Charge Atomistic Simulations

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Our previous work[1] presented a curated database of calculated and experimental hydration free energies, along with input files and structures of the molecules involved. The set ostensibly consisted of 504 molecules, but in fact contained several duplicates as we detail below, as well as errors in the identity of some of the compounds considered, and mistakes in the experimental values of others.

Here, we detail the mistakes in our original set and also refer future users of the set to the FreeSolv database,[2] available in versioned form via http://www.escholarship.org/uc/item/6sd403pz, for the authoritative version of the database previously contained in the Supporting Information of this paper.

The mistakes in our original set, detailed fully below, were not substantial enough to affect any of our overall conclusions or require recalculation of statistics on the entire set. However, since the full set including input files is deposited in the Supporting Information of our work[1] and has been used fairly widely as a basis for follow-up studies, these issues are important to note for the record.

We fully expect that as the field moves forward and does additional work curating hydration free energy data, further issues (especially with the experimental data) may be uncovered. Since journal article Supporting Information does not provide a practical means for database updates (the only means for doing so is via errata), we plan to incorporate the results of any *new* curation into new versions of the FreeSolv database rather than by submitting an erratum to this paper and making an update to the Supporting Information.

Specific issues we corrected relating to our database were as follows:

- Several molecules were present as duplicates under alternate names: 2-methylbut-2-ene and 2-methyl-but-2-ene; 3-methylbut-1-ene and 3-methyl-but-1-ene; benzonitrile and cyanobenzene; 2-methoxy-2-methylpropane and methyl-*tert*-butyl-ether. In FreeSolv, only one of each is retained.
- We also removed a duplicate butanal which had an incorrect experimental value.
- We removed "triacetyl glycerol" which was not the intended molecule (the intended molecule was "glycerol triacetate" which is still present in FreeSolv).
- We corrected the experimental value for hexafluoropropene, which had incorrectly been the value for hexafluoropropan-2-ol.
- Additional curation of experimental values was done via cross-comparison with J. Peter Guthrie's database (in preparation), resulting in updates to experimental values for 4-propylphenol, 4-bromophenol, 3-hydroxybenzaldehyde, 2-methoxyethanol, and dimethyl sulfoxide (methanesulfinylmethane).
- A number of IUPAC names were standardized.
- A small correction was made to the experimental value of 1,3-butadiene, correcting the results of a typo in the cited Hine and Mookerjee work.
- Experimental values for 2,6-dichlorosyrangaldehyde and 3,5-dichloro-2,6-methoxyphenol were updated with better-curated values.
- The experimental value for (2*E*)-hex-2-enal was corrected very slightly.

More detail on these corrections is provided in the documentation distributed with FreeSolv.[2]

In summary: None of the conclusions in our original study need revision, but the set of calculated and experimental hydration free energies provided in the Supporting Information is now obsolete and is replaced by FreeSolv (http://www.escholarship.org/uc/item/6sd403pz).

REFERENCES

(1) Mobley, D. L.; Bayly, C. I.; Cooper, M. D.; Shirts, M. R.; Dill, K. A. Small Molecule Hydration Free Energies in Explicit Solvent: an Extensive Test of Fixed-Charge Atomistic Simulations. *J. Chem. Theory Comput.* **2009**, *5*, 350−358.

(2) Mobley, D. L.; Guthrie, J. P. FreeSolv: a Database of Experimental and Calculated Hydration Free Energies, with Input Files. *J. Comput.-Aided Mol. Des.* **2014**, *28*, 711−720.

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