

Corrections

CHEMISTRY, BIOPHYSICS. For the article “Assessing implicit models for nonpolar mean solvation forces: The importance of dispersion and volume terms,” by Jason A. Wagoner and Nathan A. Baker, which appeared in issue 22, May 30, 2006, of *Proc Natl Acad Sci USA* (103:8331–8336; first published May 18, 2006; 10.1073/pnas.0600118103), the authors note that an error in the implementation of Eq. 10 in the original paper led to improper scaling of the solvent-accessible volume forces for highly exposed

surface atoms. The error in the original implementation of Eq. 10 affects Tables 1 and 2 of the original manuscript as well as Tables 3 and 4 and Figs. 2 *B* and *C* and 3 in the original supporting information. Corrected versions of Tables 1 and 2 appear below. A correction to the supporting information has been published online. This error does not affect the conclusions of the article.

Table 1. Optimized 6/12 and WCA implicit solvent nonpolar MF parameter values and goodness-of-fit metrics

| Parameters | MF model 6/12 | | | MF model WCA | | |
|---|------------------|------------------|------------------|-----------------|------------------|------------------|
| | Attractive | Repulsive | Total | Attractive | Repulsive | Total |
| σ_s , Å | 0.89 [0.87–0.91] | 1.29 [1.16–1.44] | 1.68 [1.57–1.80] | 0.8 [0.73–0.86] | 1.29 [1.18–1.41] | 1.25 [1.16–1.39] |
| γ , cal·mol ⁻¹ ·Å ⁻² | — | 15(1) | 1(1) | — | 2(1) | 0(1) |
| ρ , cal·mol ⁻¹ ·Å ⁻³ | — | 94(2) | 55(2) | — | 52(2) | 55(2) |
| r | 0.88 | 0.56 | 0.83 | 0.84 | 0.87 | 0.86 |
| R | 0.97 | 0.91 | 0.94 | 0.97 | 0.94 | 0.94 |
| χ^2 , 10 ⁻³ kcal ² ·mol ⁻² ·Å ⁻² | 6.99 | 3.35 | 6.47 | 0.56 | 4.87 | 4.63 |

Separate fits of nonpolar solvation MFs were performed as follows: Attractive, a comparison of attractive implicit (Eq. 15) and attractive explicit; Repulsive, a comparison of repulsive implicit (Eq. 10) and repulsive explicit; and Total, a comparison of the total implicit (Eq. 21) and total explicit (Eq. 8) nonpolar MFs. Where applicable, standard errors are presented in parentheses; 99% confidence intervals (see text) are presented in brackets.

Table 2. Comparison of total solvation energies (kcal/mol) for small alkane solutes

| Compound | WCA 1.25 | WCA 0.65 | OPLS | AMBER | Exp. |
|----------------|----------|----------|------|-------|------|
| Methane | 6.40 | 1.93 | 2.40 | 2.69 | 2.00 |
| Ethane | 8.41 | 2.25 | 2.63 | — | 1.83 |
| Propane | 10.5 | 2.84 | 2.89 | 3.02 | 1.96 |
| Butane | 11.8 | 2.93 | 3.21 | 3.19 | 2.08 |
| Pentane | 13.7 | 3.48 | 3.78 | — | 2.33 |
| Hexane | 15.6 | 3.90 | 3.78 | — | 2.49 |
| Isobutane | 12.0 | 3.16 | 3.03 | 3.27 | 2.52 |
| 2-Methylbutane | 13.4 | 3.45 | 3.51 | — | 2.38 |
| Neopentane | 13.2 | 3.46 | 3.23 | — | 2.50 |
| Cyclopentane | 11.3 | 2.25 | 2.80 | — | 1.20 |
| Cyclohexane | 13.7 | 3.18 | 2.34 | — | 1.23 |

WCA energy values were obtained by using the methods described in the text with $\sigma_s = 1.25$ and 0.65 Å. OPLS energies were taken from Gallicchio *et al.* (35) by using values in table 2 of their paper. AMBER energies are from Shirts *et al.* (64), ‘van der Waals’ values in table II of their paper. Experimental (Exp.) values are from table VII of Cabini *et al.* (65).

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