# Correction to A Toolkit to Fit Nonbonded Parameters from and for Condensed Phase Simulations

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# Correction to A Toolkit to Fit Nonbonded Parameters from and for Condensed Phase Simulations

Florent Hédin,[†] Krystel El Hage,[†] and Markus Meuwly[*,†,‡]

†*Department of Chemistry, University of Basel, Klingelbergstrasse 80, CH-4056 Basel,*
*Switzerland*

‡*Department of Chemistry, Brown University, Providence, Rhode Island 02912, USA.*

E-mail: m.meuwly@unibas.ch

In a recent publication we presented a fitting environment for parametrizing point charge (PC) and multipolar (MTP) force fields for condensed-phase simulations.[1] After publication of this work it came to our attention that one of the scripts contained an error which caused an energy component in the free energy simulations to return incorrect values. This affects the optimization of the parameter $\ell$ when scaling the Lennard-Jones parameters according to $\varepsilon^* = \ell\varepsilon$ and $R^*_{\min}/2 = \ell R_{\min}/2$ but not the MTP terms.

Hence, all compounds considered were reparametrized according to the procedure described in Ref.[1] The corresponding correlations between experiment and the optimized parametrizations are reported in Figures 1 and 2. While the best $\ell$ typically differs by $\Delta\ell = 0.1$ the average quality of all parametrizations is unchanged. In the published article[1] the statistical measures for $\Delta G_{\mathrm{hyd}}$ and $\Delta H$ were (RMSE=0.36 kcal/mol, $R^2 = 0.99$) and (RMSE = 0.53 kcal/mol, $R^2 = 0.97$) (see Figures 3 and 4 in Ref.[1]), which changes to (RMSE=0.31 kcal/mol,
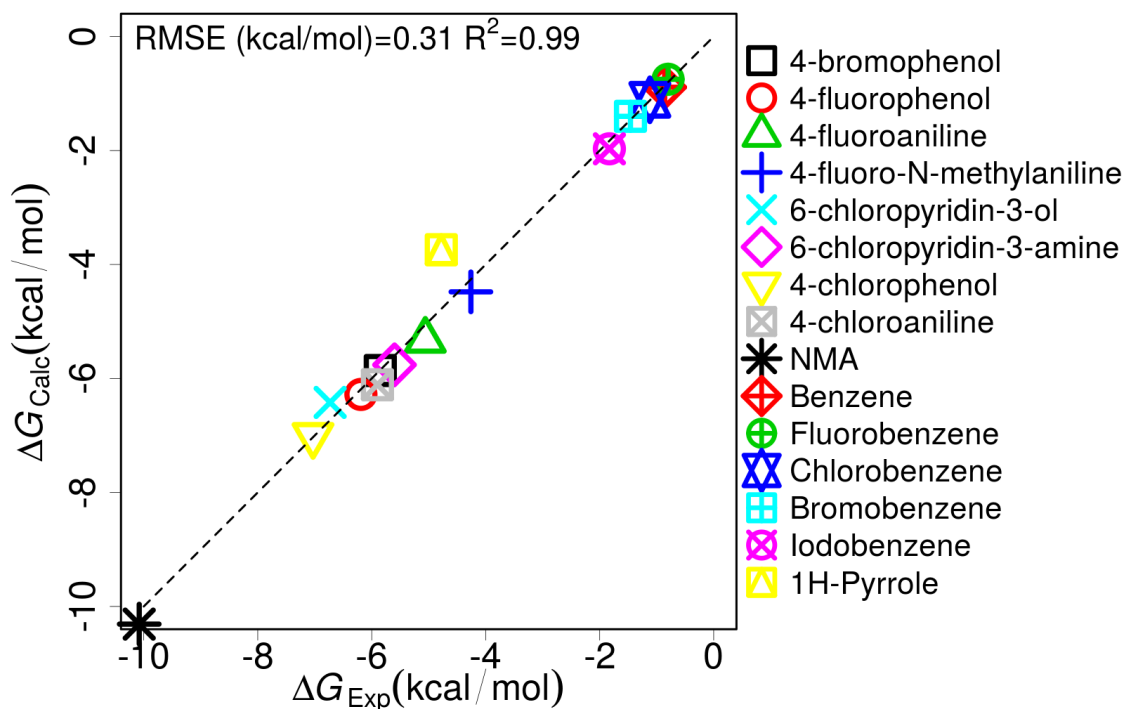
Figure 1: Correlation between experimental and computed solvation free energies $\Delta G_{\mathrm{hyd}}$ (kcal/mol, respectively, $x-$axis and $y-$axis) for a range of compounds of interest. Computed values obtained after optimization of the LJ parameters.

$R^2 = 0.99$) and (RMSE $= 0.57$ kcal/mol, $R^2 = 0.96$) using the correct script, respectively.

For one example, N-Methyl-Acetamide, the three observables $(\rho, \Delta H, \Delta G_{\mathrm{hyd}})$ were given explicitly as a function of the scaling $\ell$ in Table 1 of Ref.[1] This data has been recomputed and is reported here in Table 1. In this case the same scaling $\ell = 0.95$ is found to provide the best parametrization, i.e. the one with the lowest score $S = \sum_{i=1}^{3} w_i (\mathrm{Obs_i} - \mathrm{Calc_i})^2$ with $w_\rho = 1$, $w_{\Delta H} = 3$ and $w_{\Delta G} = 5$ which differently weights the three observables.[1] The scores $S$ are now larger in magnitude than in the original work[1] because the results from the hydration free energy simulations differ.

The current results show that the quality of the parametrizations and all conclusions from
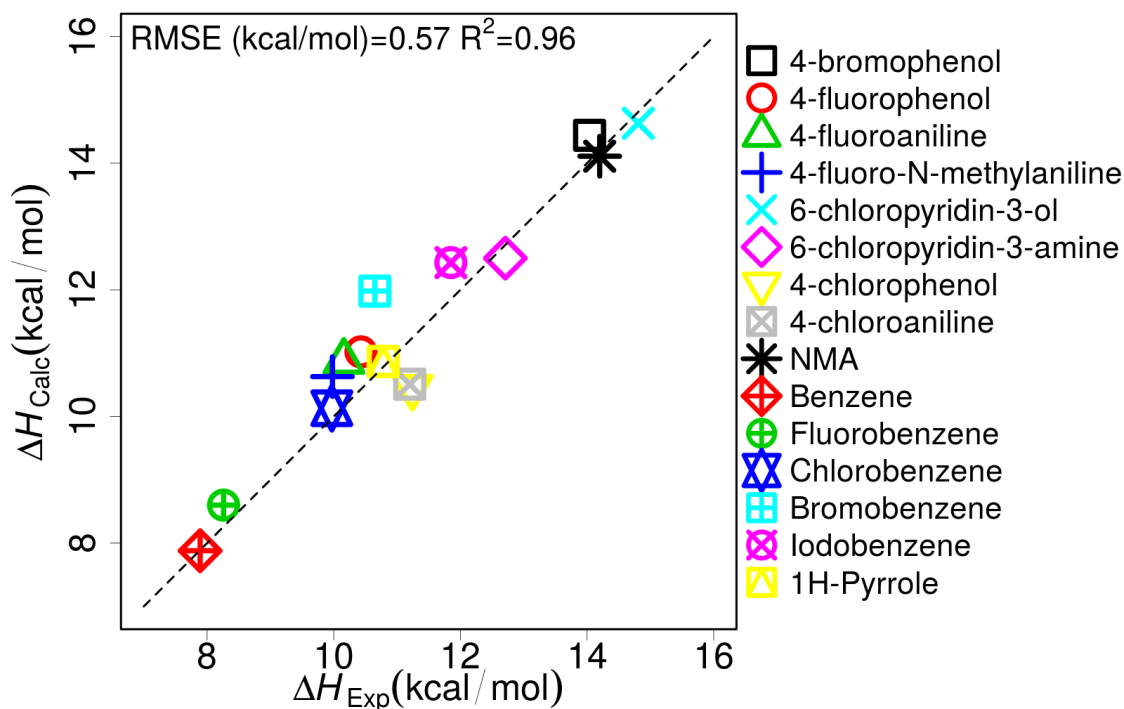
Figure 2: Correlation between experimental and computed enthalpy of vaporization $\Delta H_{\text{vap}}$ (kcal/mol, respectively, $x-$axis and $y-$axis) for a range of compounds of interest. Both, MTP and LJ parameters were optimized.

Table 1: Dependence of $\rho$ (g/cm$^3$), $\Delta H_{\text{vap}}$ and $\Delta G_{\text{hyd}}$ (both in kcal/mol) when scaling the Lennard-Jones parameters. In bold face is shown the value of $\ell$ minimising the score $S$.

| Scaling $\ell$ | $\rho$ | $\Delta H_{\text{vap}}$ | $\Delta G_{\text{hyd}}$ | Score $S$ |
|---|---|---|---|---|
| 0.9 | 1.13 | 14.24 | -10.57 | 1.2 |
| 0.925 | 1.08 | 13.95 | -10.41 | 0.8 |
| **0.95** | **1.00** | **14.11** | **-10.31** | **0.3** |
| 0.975 | 0.99 | 13.84 | -10.23 | 0.5 |
| 1 | 0.95 | 13.82 | -9.78 | 0.9 |
| 1.025 | 0.92 | 13.68 | -9.27 | 4.1 |
| 1.05 | 0.88 | 13.57 | -9.01 | 6.9 |
| 1.075 | 0.84 | 13.29 | -8.21 | 20.0 |
| 1.1 | 0.81 | 13.47 | -7.98 | 23.7 |
| Expt. | 0.94[2,3] | 14.2[2,4] | -10.08[5] | |

the original article remain unchanged. However, the value of the scaling $\ell$ that is required

for a particular quality of a parametrization changes.

# References

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