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ADDITION/CORRECTION

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Structure and Dynamics of the Aβ_{21-30} Peptide from the Interplay of NMR Experiments and Molecular Simulations
[*Journal of the American Chemical Society* **2008**, *130*, 6145–6158 DOI: 10.1021/ja710366c]. Nicolas L. Fawzi, Aaron H. Phillips, Jory Z. Ruscio, Michaeleen Doucleff, David E. Wemmer, and Teresa Head-Gordon*

Page 6151. We present the corrected experimental and predicted three-bond scalar coupling constants ($^3J_{H^NH^\alpha}$) for Aβ_{21-30} and a revised Figure 2. This correction does not change any of the other results presented in the work, nor are any of the conclusions affected. The agreement between the corrected simulation and experimental values of $^3J_{H^NH^\alpha}$ remains good (corrected Figure 2, upper panel), while the deviation from experiment of the values predicted from the minimized mean structure remains large, with $\chi^2 = 5.4$ (corrected Figure 2, lower panel).

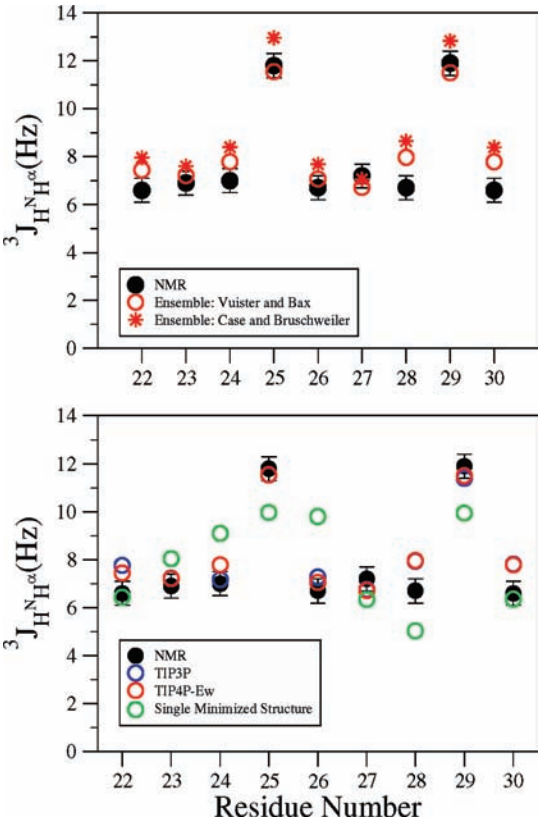

Figure 2. Comparison of experimental scalar coupling constant $^3J_{H^NH^\alpha}$ and that calculated from the simulated ensembles. Error bars are experimental uncertainty for NMR values. The coupling constants for the H^α protons of glycine are added to compare to experiment in which they are indistinguishable. (upper panel) Two parametrizations of the Karplus equation averaged over a single replica exchange ensemble by using the TIP4P-Ew model. It is apparent that the dynamically uncorrected and harmonically corrected Karplus parameter sets work equally well on this disordered system. (lower panel) Average over the two independent replica exchange ensembles for different empirical force fields and compared to experimentally determined coupling constants. It is evident that an ensemble measurement gives far better agreement with the experimental $^3J_{H^NH^\alpha}$ values than that calculated from a single structure based on incorporating all of the ROESY restraints (shown in Figure 6).

Page 6149. We also take this opportunity to correct two minor typographical errors. The coefficient for $J(\omega_H)$ was incorrect in eq 3e, which should read

$$R_2^{DD} = (1/40)K^2[4J(0) + J(\omega_H - \omega_C) + 3J(\omega_C) + 6J(\omega_H) + 6J(\omega_H + \omega_C)] \quad (3e)$$

The r_{eff} term should be cubed in eq 3f, which should read

$$K = \frac{\mu_0}{4\pi r_{eff}^3}\hbar\gamma_a\gamma_b \quad (3f)$$

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