

Dear Stephan,

Thank you for saving us from an embarrassing misuse of the uncertainty equation of Kontaxis et al. (2000). In the new version of the revised Supporting Information file, we deleted the Kontaxis reference and changed the footnote of Table S1 to a more back-of-the-envelope estimate:

“The cross-peaks of amide protons showed full linewidths at half-height of up to about 70 Hz in paramagnetic samples, while signal-to-noise ratios (S/N) typically were at least 6:1. Estimating the uncertainty of peak position as a quarter of 70 Hz yields a PCS uncertainty of 0.02 ppm. The $\Delta\chi$ -tensor fits (Figure 4) suggest that actual uncertainties were of this order of magnitude or smaller. An accurate estimate of uncertainties is complicated by the sensitivity of the chemical shifts (in particular of amide protons) to minor differences in sample conditions between paramagnetic and diamagnetic samples, the impact of which is difficult to predict.”

The peak positions were much better defined in the diamagnetic samples and any systematic shift between diamagnetic and paramagnetic samples were taken care of in the $\Delta\chi$ -tensor fitting routine.

Best regards,
Gottfried