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CORRECTION

Correction to: Characterization of fibril dynamics on three timescales by solid-state NMR

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In our recent publication (Smith et al. 2016) on the dynamics of HET-s(218–289), we reported on page 176, that calculation of solid-state NMR $R_{1\rho}$ rate constants using analytical equations based on Redfield theory (Kurbanov et al. 2011) failed when the correlation time of motion becomes too long. We have realized since then that this statement is not correct. What we did not fully consider is the fact that $R_{1\rho}$ relaxation in solid-state NMR is multi-exponential, due to different orientations of the sample in the rotor. In our original analysis, we simulated $R_{1\rho}$ relaxation both in the lab frame and rotating frame, and averaged the time-dependent magnetization decays from all orientations in a first step, and subsequently fitted the resulting sum magnetization decay to a mono-exponential function in order to extract the $R_{1\rho}$ rate constants. Because this average magnetization decay is multi-exponential, imperfect fits to a mono-exponential function led to disagreement between simulation and analytical equations - especially where $R_{1\rho}$ reaches a maximum, and becomes both larger and more strongly multi exponential. In Fig. 1, which should replace Fig. 3 of the original manuscript, we show that if one fits each orientation to extract the orientation-specific relaxation-rate constant and in a second step, averages those rate constants, simulation and analytical equations agree very well.

For the relaxation analysis presented in the paper and the numerical values of order parameters and correlation times calculated, this correction has no influence.

We would like to thank Alexey Krushelnitsky and Kay Saalwächter for raising this question and helping us sort out the correct treatment for $R_{1\rho}$ data.

Kurbanov R, Zinkevich T, Krushelnitsky A (2011) The nuclear magnetic resonance relaxation data analysis in solids: General R 1/R 1 equations and the model-free approach. J Chem Phys 135:184104:(184101–184109)

Smith AA, Testori E, Cadalbert R, Meier BH, Ernst M (2016) Characterization of fibril dynamics on three timescales by solid-state NMR. J Biomol NMR 65:171–191

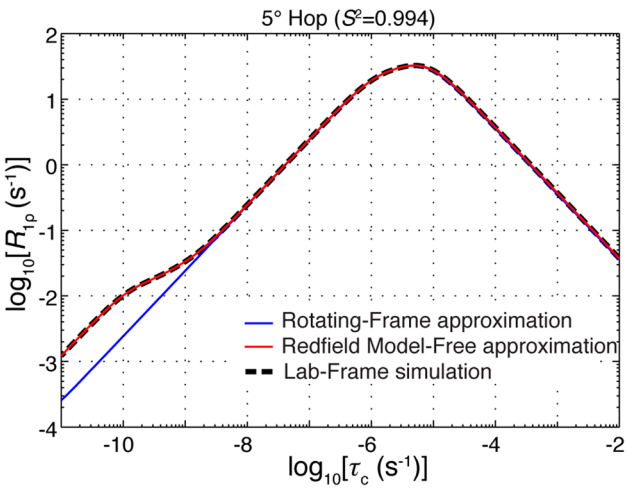

Fig. 1 Comparison of $R_{1\rho}$ calculation methods. We calculate $R_{1\rho}$ for a ^{1}H–^{13}C spin system with $\delta^{IS}/2\pi = 46.6$ kHz, $\omega_r/2\pi = 60$ kHz, and $\omega_1/2\pi = 35$ kHz, undergoing a hopping motion between two orientations, separated by 5°. The correlation time of this motion is swept. A simulation is performed in the lab-frame (*black, dotted line*), in the rotating frame (*blue line*), and a calculation is done using the model-free approach. Note that for the simulations, each different crystal orientation is fitted to a decaying exponential function, and the resulting rate constants are averaged together- in contrast to our previous approach

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