Supporting Information: Rotational dynamics of proteins from spin relaxation times and molecular dynamics simulations

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S1 Supplementary Figures

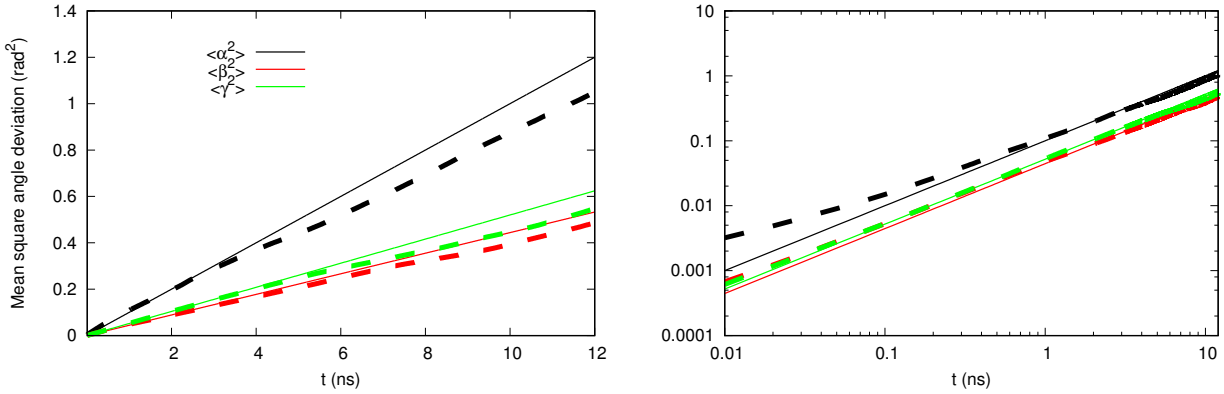

Figure S1: Mean square angle deviations of inertia tensor axes calculated from *Pa*TonB-96 simulation with tip4p water model at 310K. The data shown with linear (left) and logarithmic scale (right).

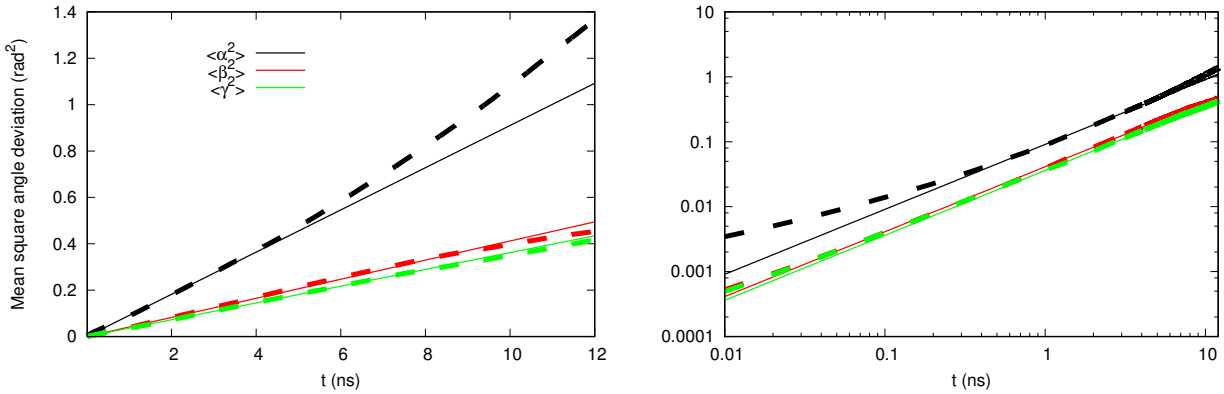

Figure S2: Mean square angle deviations of inertia tensor axes calculated from *Pa*TonB-96 simulation with tip4p water model at 298K. The data shown with linear (left) and logarithmic scale (right).

Table S1: Scaling factors of rotational diffusion for different proteins simulated with different water models. The last row shows the ratio of simulated and experimental water self-diffusion constant.

	tip3p	tip4p	OPC4
*Hp*TonB-92	2.9	1	-
*Pa*TonB-96	-	1.2	-
Calcium recoverin[1]	3.2	-	-
CBM-64[2]	-	-	1.3
65K C-RRM[3]	-	1	-
Water self-diffusion[4]	2.4	1.1	1

References

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(2) Heikkinen, H. A.; Iwai, H. In Preparation.

(3) Norppa, A. J.; Kauppala, T. M.; Heikkinen, H. A.; Verma, B.; Iwai, H.; Frilander, M. J. Mutations in the U11/U12-65K protein associated with isolated growth hormone deficiency lead to structural destabilization and impaired binding of U12 snRNA. 2017; `10.1261/rna.062844.117`.

(4) Izadi, S.; Anandakrishnan, R.; Onufriev, A. V. Building Water Models: A Different Approach. *J. Phys. Chem. Lett.* **2014**, *5*, 3863–3871.