Supplementary information for

Accelerated ^{19}F biomolecular magic-angle spinning NMR with paramagnetic dopants

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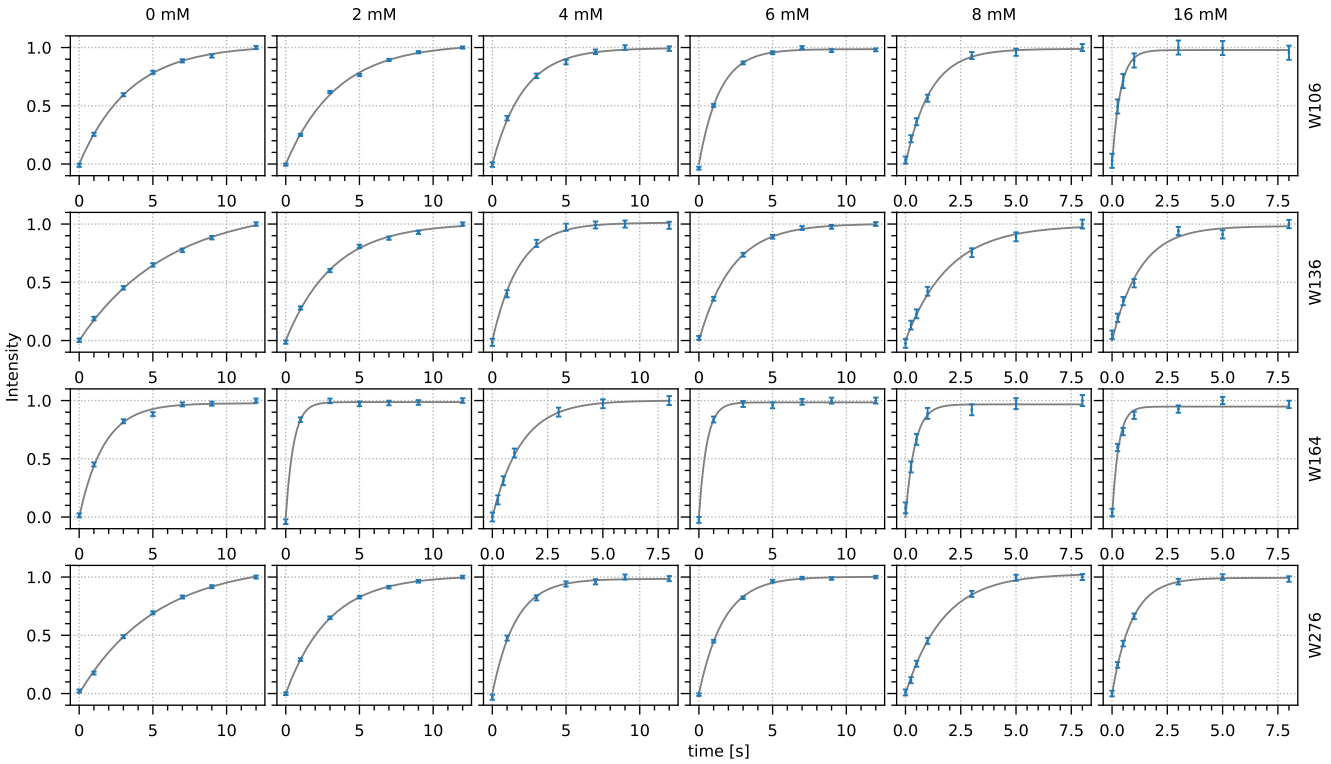

Figure S1: Residue-wise exponential fits of ^{19}F R_1 saturation-recovery relaxation experiments (Fig. 1b) at seven different concentrations of Gd(DTPA-BMA). Concentrations and residues are indicated on the top and at the right side, respectively.

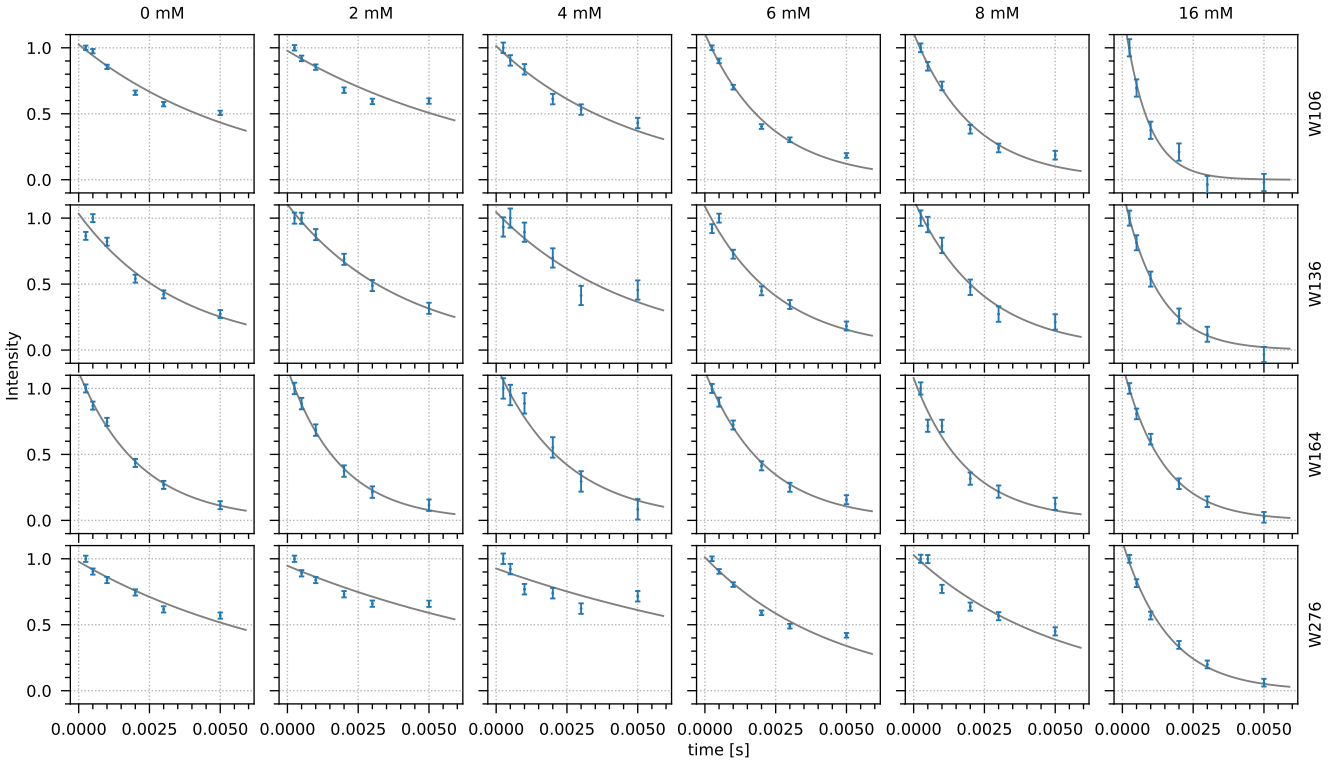

Figure S2: Residue-wise exponential fits of ^{19}F R_2 relaxation experiments (Fig. 1c) at seven different concentrations of Gd(DTPA-BMA). Concentrations and residues are indicated on the top and at the right side, respectively.

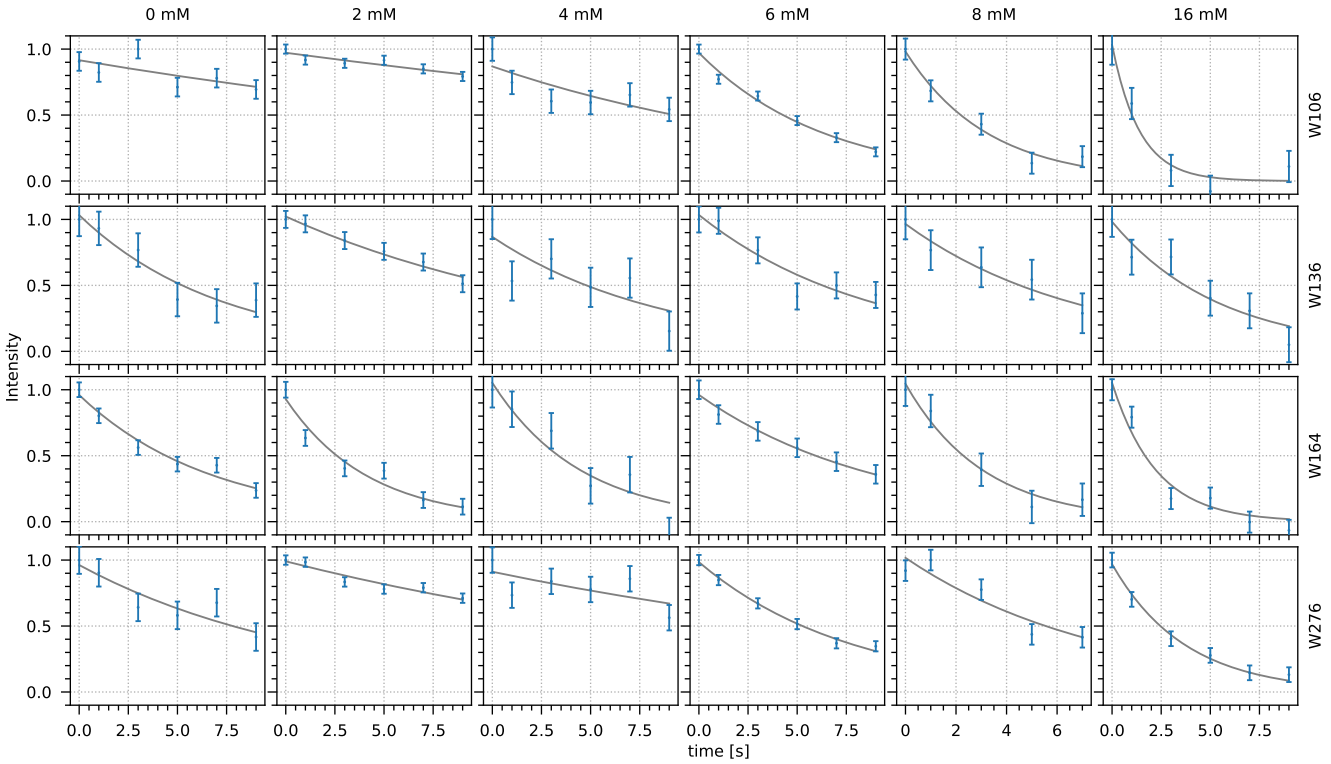

Figure S3: Residue-wise exponential fits of ^{13}C R_1 relaxation experiments (Fig. 1d) at seven different concentrations of Gd(DTPA-BMA). Concentrations and residues are indicated on the top and at the right side, respectively.

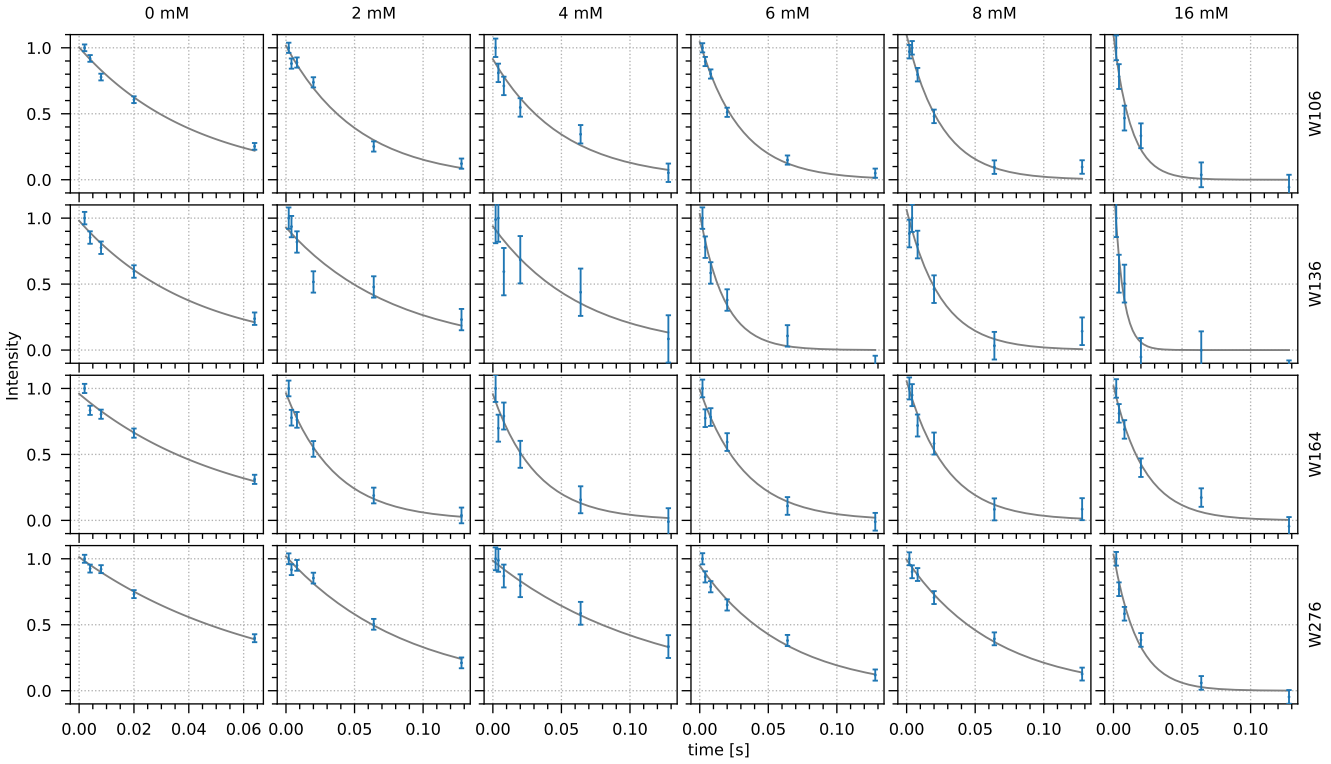

Figure S4: Residue-wise exponential fits of ^{13}C R_2 relaxation experiments (Fig. 1e) at seven different concentrations of Gd(DTPA-BMA). Concentrations and residues are indicated on the top and at the right side, respectively.

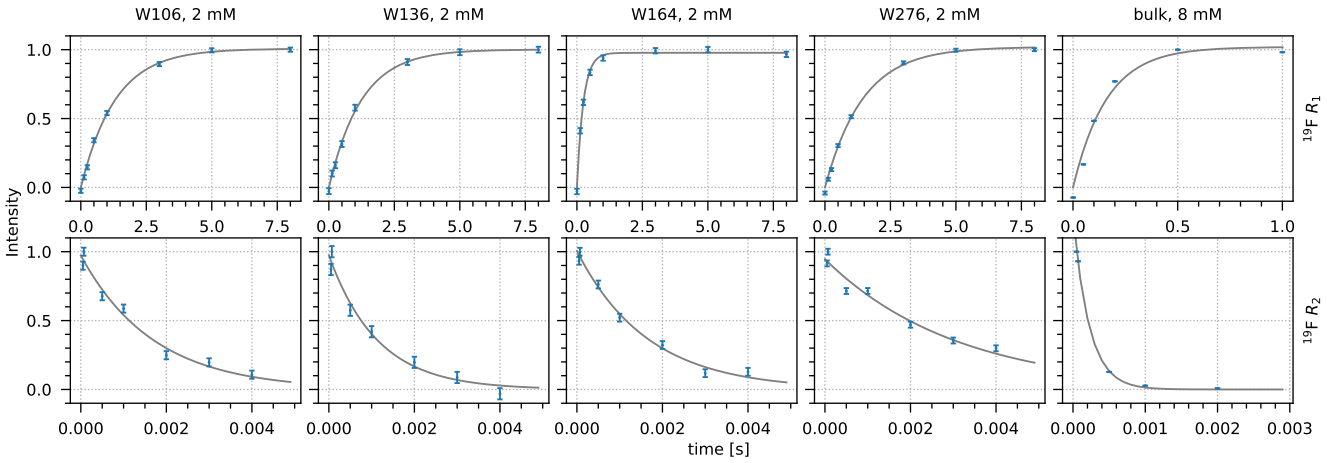

Figure S5: Exponential fits of ^{19}F R_1 (top) and R_2 (bottom) relaxation experiments (Fig. 1b,c) at two different concentrations of Gd(DTPA). The first four columns are residue-wise fits at 2 mM Gd(DTPA). The last column is a fit of the bulk signal at 8 mM Gd(DTPA), as the signals were not resolved due to broadening.

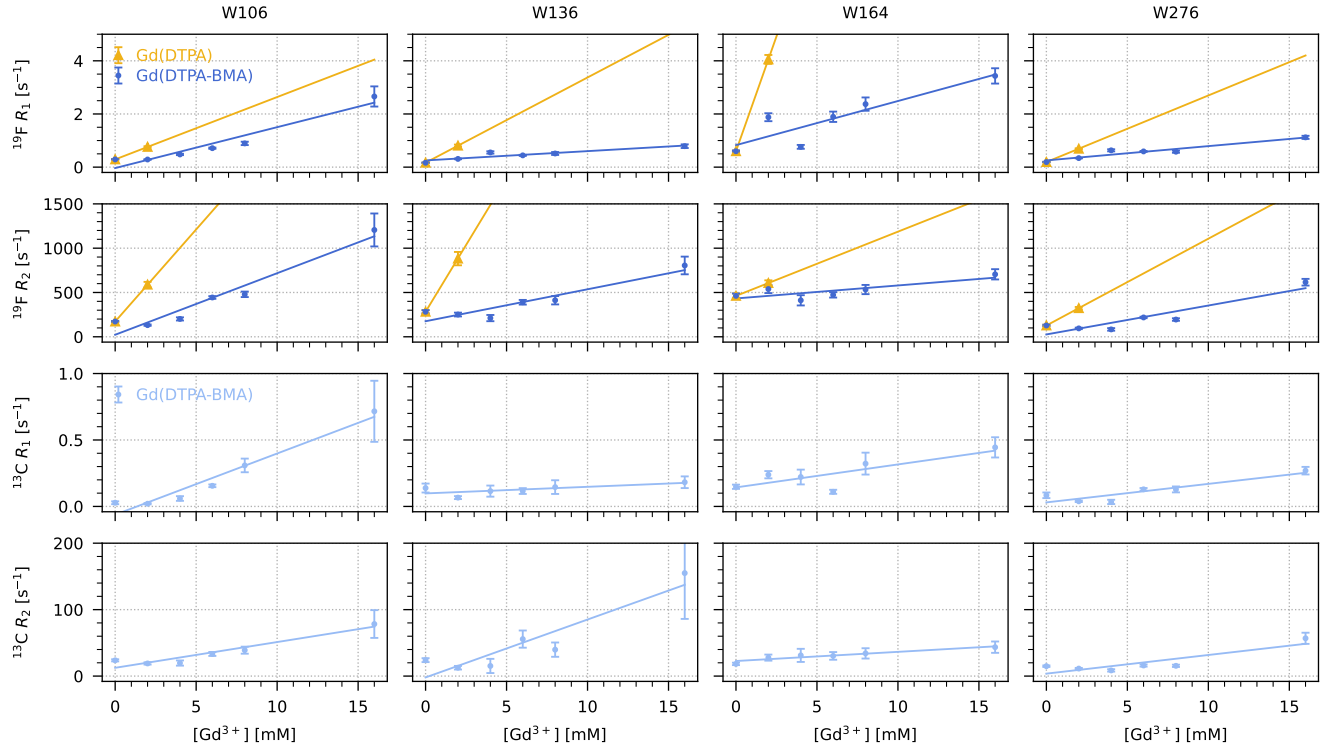

Figure S6: Linear fits of ^{19}F and ^{13}C R_1 and R_2 relaxation rates (see y-axis labels) as a function of the concentration of Gd(DTPA-BMA) and Gd(DTPA) for each tryptophan (indicated on the top).

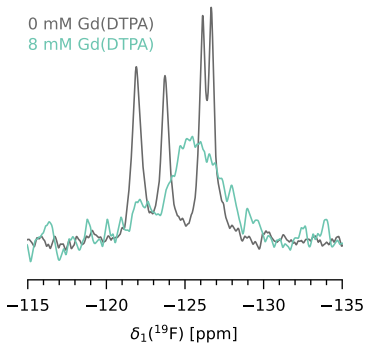

Figure S7: 1D ^{19}F MAS NMR spectrum of 5FC-W-TET without (gray) and with 8 mM Gd(DTPA) (cyan).

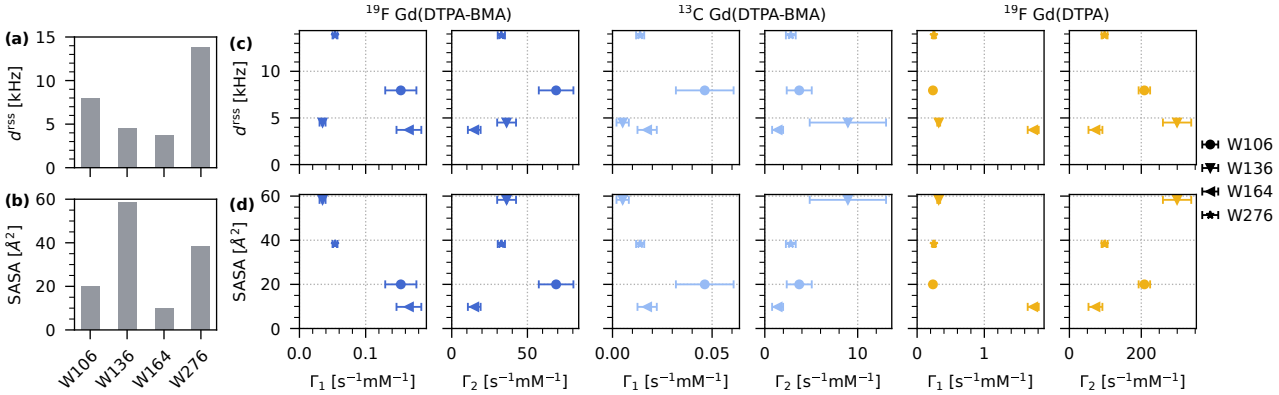

Figure S8: Analysis of tryptophan environments in TET2. (a) Strength of the dipolar coupling network d^{rss} for each tryptophan. All exchangeable protons and all protons of phenylalanines and tyrosines were considered, and distances for the calculations were based on PDB ID 1Y0R ((*1*)). (b) Surface accessible surface area (SASA) of tryptophans. The SASA was determined with the gmx sasa function implemented in GROMACS 2023.5 ((*2*)) with a probe radius of 1.4 nm. (c) Correlations between d^{rss} and Γ_1 and Γ_2. (d) Correlations between SASA and Γ_1 and Γ_2.

References

(*1*) Borissenko, L., and Groll, M. (2005). Crystal structure of TET protease reveals complementary protein degradation pathways in prokaryotes. *J. Mol. Biol. 346*, 1207–1219.

(*2*) Abraham, M. J. et al. (2015). GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers. *SoftwareX 1-2*, 19–25.