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ADDITIONS AND CORRECTIONS

Characterization of the FKBP·Rapamycin·FRB Ternary Complex [*J. Am. Chem. Soc.* **2005**, *127*, 4715−4721]. Laura A. Banaszynski, Corey W. Liu, and Thomas J. Wandless*

Supporting Information, pages S17−S18. The ^{15}N and ^{1}H chemical shifts of the backbone amides for the sequential assignment of FRB reported in this manuscript were inadvertently mis-stated by one register. The chemical shifts of the C-alpha (CA) and C-beta (CB) atoms are correct as originally reported. The Supporting Information has been changed to reflect the correct assignments.

Page 4719. Figure 5 and its caption have been updated (below) to reflect the correct sequence assignment. [See the published full paper for references cited in the caption.]

Supporting Information Available: Supporting figures; experimental details for the synthesis of rapamycin derivatives and spectra of the compounds; partial differential equations used to fit competition binding data for dissociation constants; additional details regarding SPR experiments; chemical shift assignments for FRB backbone residues (corrected). This material is available free of charge via the Internet at http://pubs.acs.org.

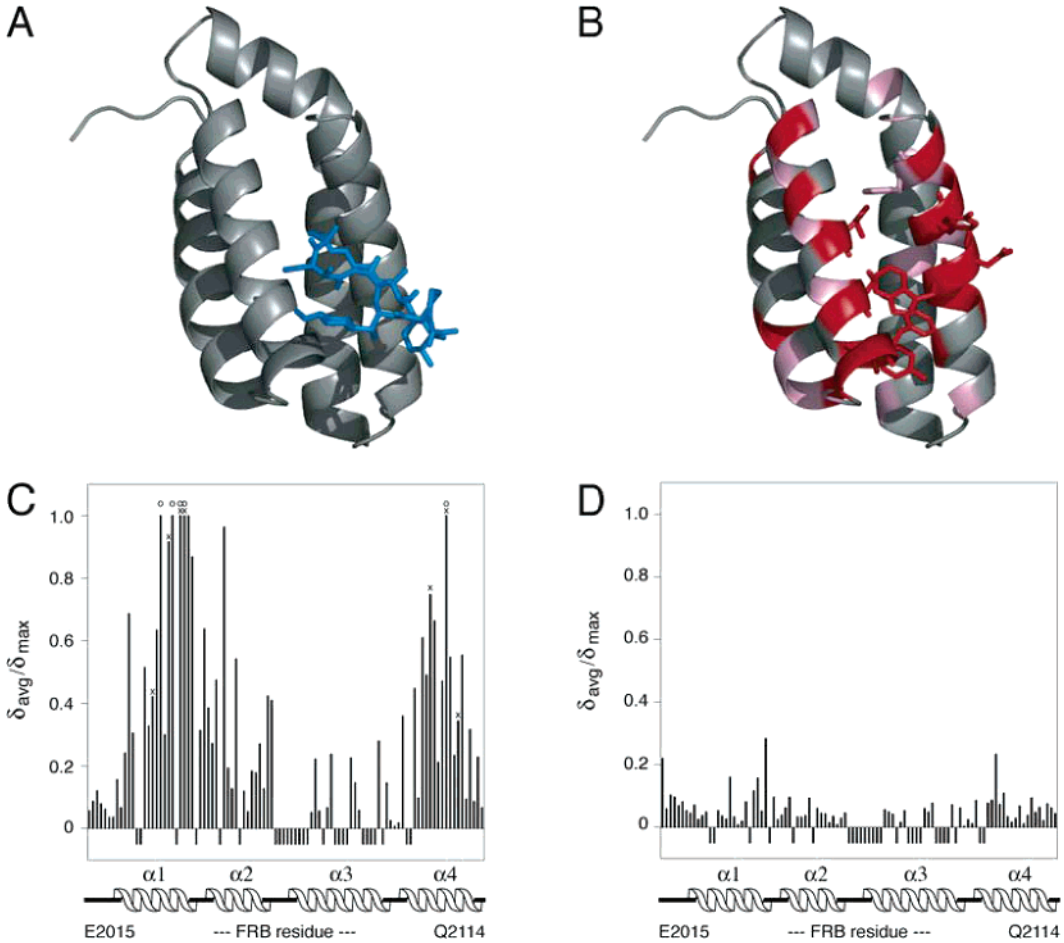

Figure 5. Effects of rapamycin and TMOP−rapamycin titrations on backbone ^{1}H and ^{15}N chemical shifts of FRB. Perturbations are displayed as normalized weighted average shift differences, $\delta_{avg}/\delta_{max}$ (see Experimental Procedures). All experiments are normalized with respect to the residue that showed the greatest perturbation in chemical shift (G2040) from the rapamycin·FRB titration. Unassigned resonances are indicated as such by a negative chemical shift difference. Ribbon representations were created using PyMOL.[37] (A) Ribbon representation of FRB showing the rapamycin binding site (adopted from the FKBP·rapamycin·FRB crystal structure, 1FAP).[24] Rapamycin is shown in blue. (B) FRB ribbon representation showing residues affected by the rapamycin titration. Side chains of residues that make van der Waals contacts with rapamycin are shown. Residues experiencing strong chemical shift perturbations ($\delta_{avg}/\delta_{max} > 0.4$) are shown in red and residues experiencing moderate chemical shift perturbations ($0.2 < \delta_{avg}/\delta_{max} < 0.4$) are shown in pink. Rapamycin has been omitted for clarity. (C) Chemical shift perturbations for the rapamycin·FRB titration are plotted as a function of residue number. Residues that make van der Waals contacts with rapamycin (L2031, S2035, Y2038, F2039, W2101, Y2105, and F2108) are indicated as such (×). The resonances for E2033, R2036, Y2038, F2039, and Y2105 (denoted with an ○) broaden and become unobservable upon addition of rapamycin. These five residues have been assigned a value of 1. Secondary structure is indicated at the bottom of the graph. (D) Chemical shift perturbations for the TMOP−rapamycin·FRB titration are plotted as a function of residue number.

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