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Letters to the Editor

^{1}H, ^{13}C and ^{15}N resonance assignments of URNdesign, a computationally redesigned RRM protein

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Protein design represents one of the great challenges of computational structural biology. The ability to successfully design new proteins would allow us to generate new reagents and enzymes, while at the same time providing us with an understanding of the principles of protein stability. Here we report ^{1}H, ^{15}N and ^{13}C resonance assignments of a redesigned U1A protein, URNdesign. U1A has been studied extensively by our group and hence was chosen as a design target. For the assignments we sued 2D and 3D heteronuclear NMR experiments with uniformly ^{13}C, ^{15}N-labeled URNdesign. The assignments for the backbone NH, CO, C_{α} and C_{β} nuclei are 94% complete. Sidechain ^{1}H and ^{13}C, aromatic and Q/N NH_2 resonances are essentially complete with guanidinium and K NH_3 residues unassigned. BMRB deposit with accession number 6493.

References: Allain et al. (1996) *J. Mol. Biol.*, **257**, 398–411; Dantas et al. (2003) *J. Mol. Biol.*, **332**, 449–460.

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Backbone and side-chain ^{1}H, ^{15}N and ^{13}C assignments for the *cis* conformer of the β domain of the bacterial cell division protein DivIB

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DivIB is a vital component of the divisome, a macromolecular assembly of proteins responsible for coordinating the process of bacterial cytokinesis (Robson et al., 2002). The extracytoplasmic region of DivIB comprises three structurally autonomous domains denoted α, β, and γ from N- to C-terminus. During the process of making sequence-specific resonance assignments for the β domain of *Geobacillus stearothermophilus* DivIB (Gste-DivIBβ) we noted a dynamic equilibrium between two discrete conformers due to *cis–trans* isomerization of the Y221–P222 peptide bond. These conformers are in slow exchange on the NMR timescale, resulting in two sets of chemical shifts for ~18% of all ^{1}H, ^{15}N, and ^{13}C nuclei. Some of these chemical shift differences are dramatic, such as an 11.8 ppm difference for the ^{15}N nucleus of A223 proximal to the isomerization site. We recently published near-complete chemical shift assignments for the *trans* isomer of Gste-DivIBβ (Robson et al., 2004). Here we report complete backbone and sidechain ^{1}H, ^{15}N and ^{13}C assignments for the *cis* conformer with the exception of $^{1}H_N$ and ^{15}N nuclei of Q213, aromatic ^{13}C resonances, and the labile protons of lysine and arginine residues and their associated side-chain ^{15}N. ^{13}C' assignments have been made for all residues. The *cis* and *trans* assignments have been deposited in the BMRB database (Accession No. 6395).

References: Robson et al. (2002) *Mol. Microbiol.*, **44**, 663–674; Robson et al. (2005) *J. Biomol. NMR*, **31**, 261–262

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