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## NMR Study on the Internal Dynamics of Ketosteroid Isomerase

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The backbone dynamics of ketosteroid isomerase, a homodimeric enzyme with 125 amino acid residues per subunit, has been studied in the presence/absence of a steroid ligand and 5% trifluoroethanol (TFE) by  $^{15}$ N relaxation measurements. The relaxation data were analyzed using the model-free formalism to extract the model-free parameters ( $S^2$ ,  $\tau_e$ , and  $R_{ex}$ ). The results show that a large number of the residues, particularly those involved in the dimer interaction, exhibit reduced order parameters ( $S^2$ ) in the steroid-bound enzyme, indicating the increased high-frequency (picoto nanosecond) motions in the interface region upon ligand binding. The results also show that that the presence of 5% TFE in free enzyme causes little change or slight increase in the order parameters for a number of residues in the dimer interface region. However, the majority of the residues in free enzyme exhibit reduced order parameters in the presence of 5% TFE, indicating that the increase in entropy is partially responsible for the increased stability of KSI by 5% TFE.