



All chemical shifts are referenced to DSS

XX ← Average Chem. Shift (ppm)<sup>b</sup>  
 (XX,XX) ←  $\beta$ -sheet average chem. shift (ppm)<sup>c</sup>  
 ←  $\alpha$ -helix average chem. shift (ppm)<sup>c</sup>

<sup>a</sup> Cys in Oxidized form

<sup>b</sup> From the restricted chemical shift database of BMRB

<sup>c</sup> From Chemical Shift Index (referenced to DSS by  $\Delta\delta=2.5\text{ppm}$ )  
 The <sup>13</sup>C chemical shift index. A simple method for the identification of protein secondary structure using <sup>13</sup>C chemical shift data. Wishart, D.S. and B.D. Sykes. J. Biomol. NMR 4:171-180 (1994).

Nomenclature:

"Recommendations for the Presentation of NMR Structures of Proteins and Nucleic Acids"  
 L. Markley, A. Bax, Y. Arata, C. W. Hilbers, R. Daptein, B. D. Sykes, P. E Wright, and K. Wüthrich  
 Pure & Appl. Chem. 70, 117-142 (1998)