Supporting Materials

# Elucidation of Structural Restraints for Phosphate Residues with Different Hydrogen Bonding and Ionization States

*J. Gajda[1], S. Olejniczak[1], I. Bryndal[2] and M. J. Potrzebowski[1]**

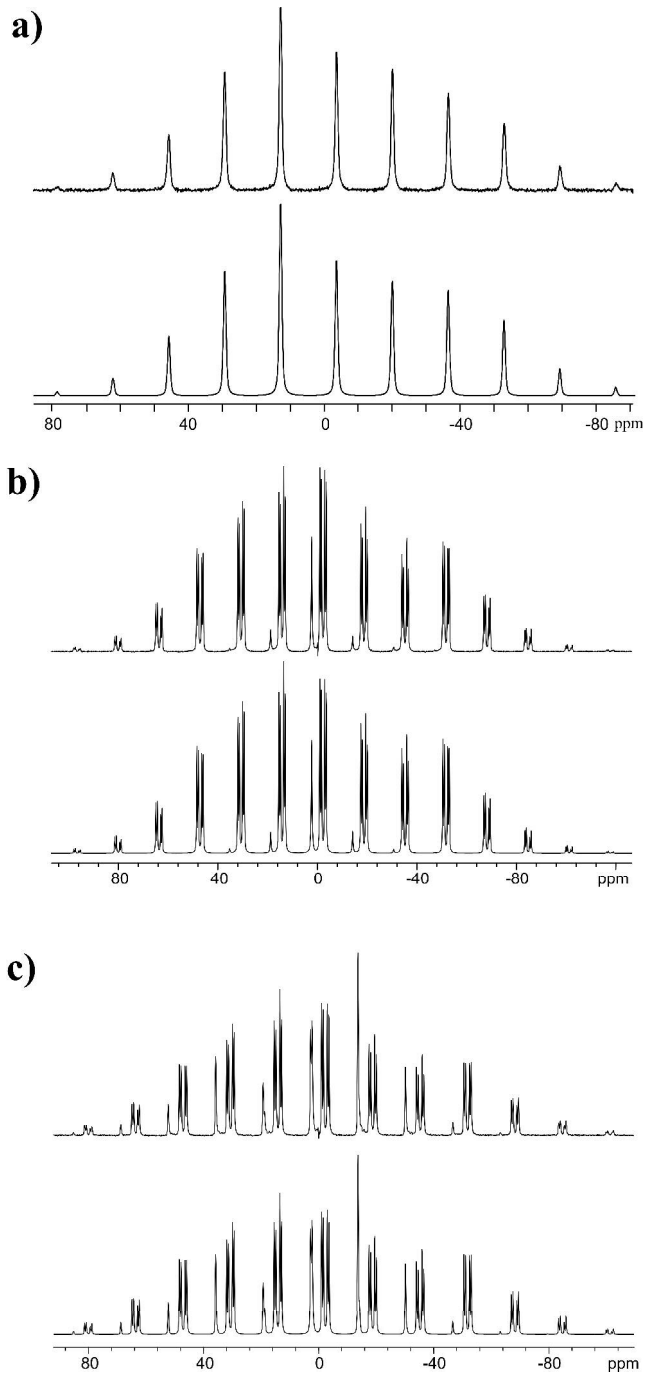


**Figure 1S.** The 31P CP/MAS spectra recorded wtih a spinning rate of 2kHz. a) O-phospho-L-threonine **1**, b) ammonium salt of O-phospho-L-threonine **2**, c) mixture of ammonium and diammonium salts of O-phospho-L-threonine **2** and **3**. Experimental spectra are presented on the top and the appropriate fitted spectra obtained employing the SIMPSON program (below).

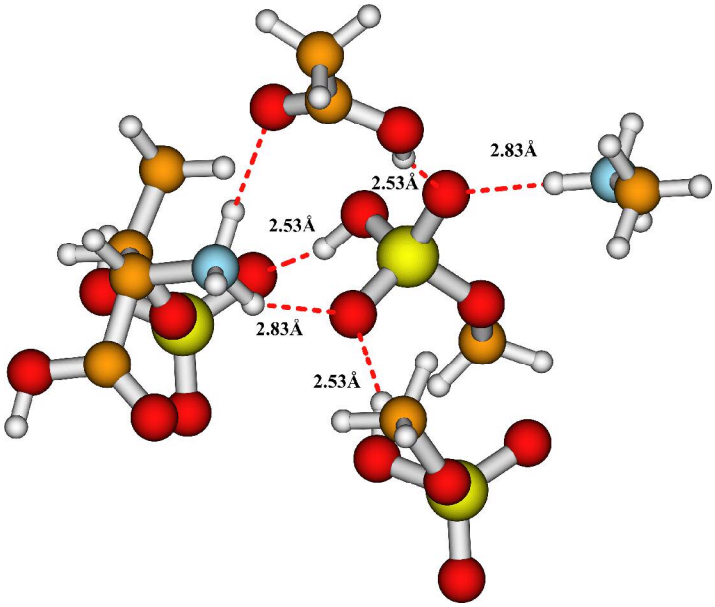


**Figure 2S.**The distances between heavy atoms involved in hydrogen bonds formed by the phosphate group (central molecule) of every independent molecule existing in one asymmetric unit of L-PThr are given in angstroems. Dotted lines show hydrogen bonds. For easier visualization, the threonine chains are replaced by $CH_3$ groups in this illustration.