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Determining the structural dynamics of MMP-3/TIMP complex from NMR relaxation

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MMP-3, or Stromelysin 1, is an proteolytic enzyme of the extracellular matrix that is involved in the repair of wounds. It is implicated in inflammation and cartilage damage and inflammation in rheumatoid arthritis and damage to the blood-brain barrier immediately after stroke. While a natural inhibitor does exist, it stops all processes, good and bad. MMP-3 must be selectively inhibited, and for this reason, we must understand how Tissue Inhibitor of Metalloproteinases (TIMP) inhibits MMP-3. Using NMR spectroscopy, the chemical shift of the ^{15}N and ^1H atoms, as well as the ^{15}N NMR relaxation data (R_1 , R_2 , and heteronuclear NOE) of the MMP-3 protein was recorded. Using NMRpipe, this data was converted into a spectrum, showing the contoured peaks. Using the NMR program Sparky, the relaxation data were fitted, and converted into a relaxation rate constant for each residue. For more accurate results, the data was filtered twice: coarse and fine. After coarse filtering, it was realized that the R_2 data were collected at different a frequency than the R_1 data. This renders the data less compatible. Preparation of new samples to be done at the correct frequencies will be completed sometime in the near future. Once this is accomplished, the new relaxation data for R_2 can be calculated, and the dynamics of the MMP-3/TIMP complex can be calculated accurately.