Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Gas-Phase Folding of Small Glutamine Containing Peptides: Sidechain Hydrogen Bonding Stabilizes β-turns. PATRICK S. WALSH[1], University of Pennsylvania, KARL N. BLODGETT, Purdue University, CARL MCBURNEY, SAMUEL H. GELLMAN, University of Wisconsin-Madison, TIMOTHY S. ZWIER, Purdue University — Glutamine is vitally important to a class of neurodegenerative diseases called poly-glutamine (poly-Q) repeat diseases such as Huntington's Disease (HD). Recent studies have revealed a pathogenic pathway that proceeds through misfolding of poly-Q regions into characteristic β-turn/β-hairpin structures that are highly correlated with toxicity. The inherent conformational preferences of small glutamine containing peptides (Ac-Q-Q-NHBn and Ac-A-Q-NHBn) were studied using conformation-specific IR and UV spectroscopies, with the goal of probing the delicate interplay between three competitive hydrogen bonding motifs: backbone-backbone, sidechain-backbone, and sidechain-sidechain hydrogen bonds. Laser desorption, coupled with a supersonic expansion, was used to introduce the non-thermally labile sample into the gas-phase. Resonant ion-dip infrared (RIDIR) spectroscopy is a powerful tool for recording the vibrational spectra of single conformational isomers and was used here to reveal the innate structural preferences of the glutamine containing peptides. Experimental results are compared against density functional calculations to arrive at firm conformational assignments. Our results demonstrate a striking preference for β-turn formation in the non-polar environment of the gas-phase.

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Date submitted: 06 Dec 2016 Electronic form version 1.4