Supplementary Information for:

Conformation-specific spectroscopy of capped, gas-phase Aib oligomers:

Tests of the Aib residue as a $3_{10}$-helix former

Joseph R. Gord$^a$, Daniel M. Hewett$^a$, Alicia O. Hernandez-Castillo$^a$, Karl N. Blodgett$^a$, Matthew C. Rotondaro$^b$, Adalgisa Varuolo$^b$, Matthew A. Kubasik$^b$, *, and Timothy S. Zwier$^a$, *

$^a$Department of Chemistry, Purdue University, West Lafayette, Indiana 47901 USA.

$^b$Department of Chemistry and Biochemistry, Fairfield University, Fairfield, Connecticut 06824 USA

KEYWORDS: Peptide folding, Helix Macrodipole, $3_{10}$-Helices, Single-conformation spectroscopy
Figure S1: Presented here are the two lowest energy fits for conformer A of Z-(Aib)$_4$-OMe. Both structures adopt F-F-10-10 conformations. The splittings between individual transitions have been given in wavenumbers. The primary structural difference between the two is incorporation of the Schellman Motif$^{29}$ in the lower energy structure. Because of the energetic and spectroscopic similarity, we do not make a definitive assignment. However, the +3.5 kJ/mol structure is favored based on slightly better spectroscopic agreement.