

Description of Additional Supplementary Files

File name: Supplementary Data 1

Description: The ¹H NMR resonance assignment, coupling patterns and coupling constants of the AcNGXA-NH₂ peptides together with the display of spectra.

File name: Supplementary Data 2

Description: The input parameters, input and output coordinates and absolute energies of the structures used in IRC path calculations and NBO analysis.

File name: Supplementary Data 3

Description: GnuPlot scripts and the corresponding source data text files.

File name: Supplementary Data 4

Description: The COPASI inputs and the corresponding data files for the kinetic model calculations.