Detection and characterization at nM concentration of oligomers formed by hIAPP, Ab(1–40) and their equimolar mixture using SERS and MD simulations.

Luisa D’Urso, Marcello Condorelli, Orazio Puglisi, Carmelo Tempra, Fabio Lolicato, Giuseppe Compagnini, and Carmelo La Rosa

a. Department of Chemical Sciences, V.le A. Doria 6 – 95125 Catania, Italy. Email: clara@unict.it
b. Department of Physics, University of Helsinki, P.O. Box 64, FI-00014 Helsinki, Finland.
c. Laboratory of Physics, Tampere University of Technology, P.O. Box 692, FI-33101 Tampere, Finland
Figure S1. Secondary structures evolution over 1 µs of atomistic simulation of first run of Aβ (1-40) and hIAPP tetramer molar ratio 1:1. Residue from 1 to 80 indicate the Aβ (1-40), the residue from 81 to 154 indicate the hIAPP residue.
Figure S2. Secondary structures evolution over 1 μs of atomistic simulation of second run of Aβ (1-40) and hIAPP tetramer molar ratio 1:1. Residue from 1 to 80 indicate the Aβ (1-40), the residue from 81 to 154 indicate the hIAPP residue.
Figure S3. Secondary structures evolution over 1 μs of atomistic simulation of third run of Aβ (1-40) and hIAPP tetramer molar ratio 1:1. Residue from 1 to 80 indicate the Aβ (1-40), the residue from 81 to 154 indicate the hIAPP residue.

Fig S4. SERS spectra of equimolar mixture of Aβ (1-40) and hIAPP at 10nM concentration. Panel in the right corner is the magnification of the amide II bands. The β-sheet/random coil ratio was calculated from the ratio between the intensity at 1568 cm\(^{-1}\) (β-sheet) and intensity at 1561 cm\(^{-1}\) (random coil).