Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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

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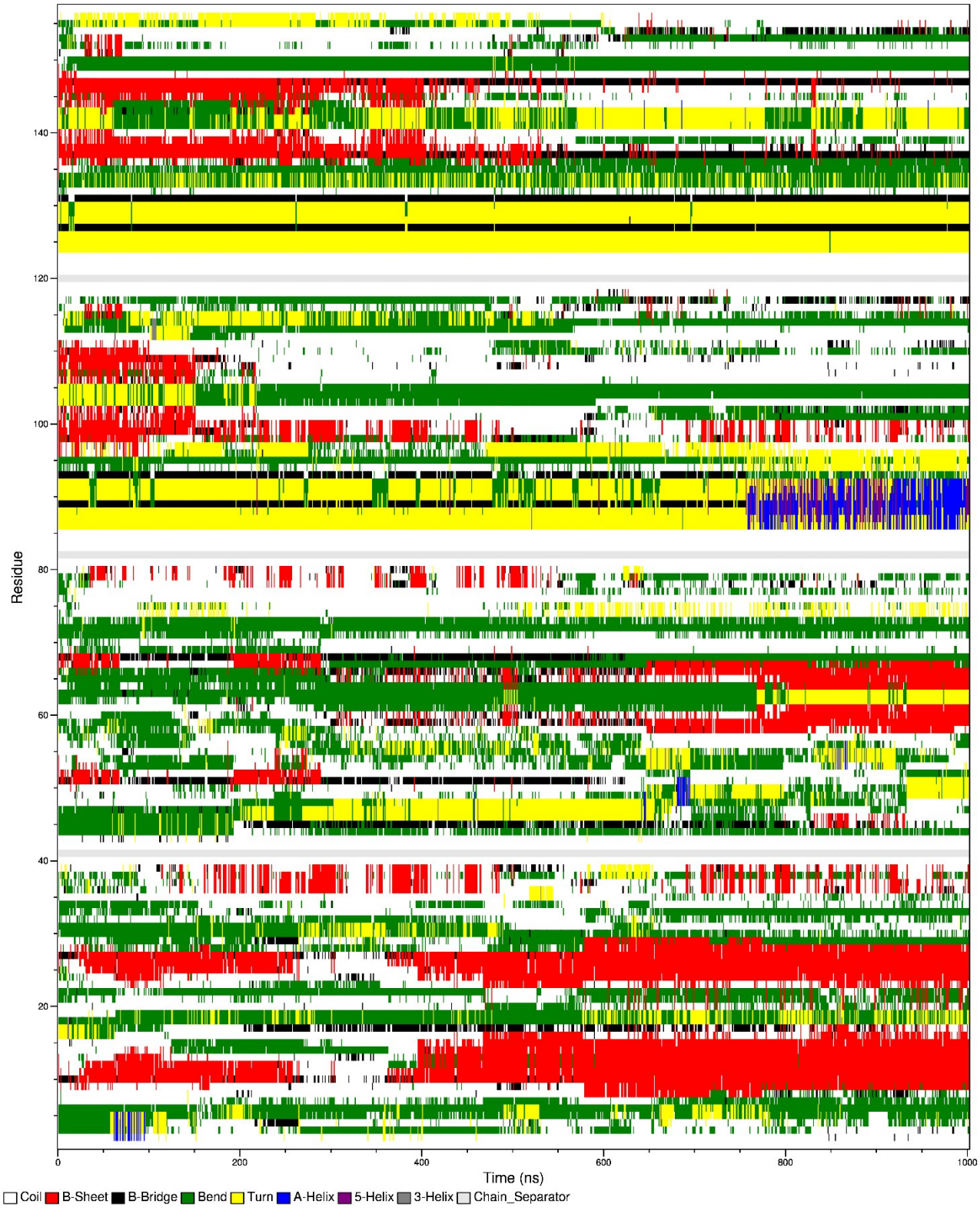

Figure S1. Secondary structures evolution over 1 μs of atomistic simulation of first run of Aβ (1-40) and hIAPP tetramer molar ratio 1:1. Residue from 1 to 80 indicate the Aβ (1-40), the residue from 81 to 154 indicate the hIAPP residue.

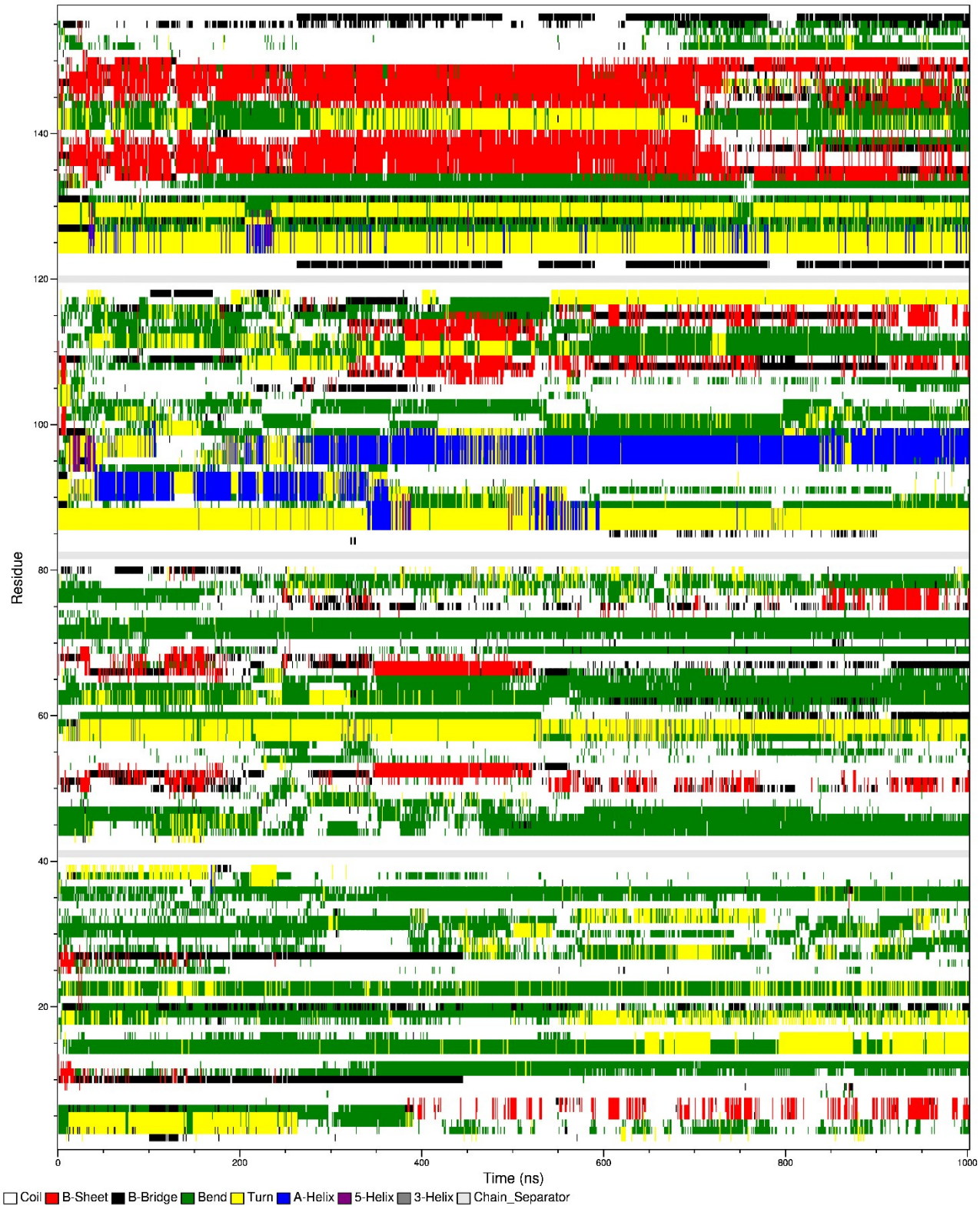

Figure S2. Secondary structures evolution over 1 μs of atomistic simulation of second run of Aβ (1-40) and hIAPP tetramer molar ratio 1:1. Residue from 1 to 80 indicate the Aβ (1-40), the residue from 81 to 154 indicate the hIAPP residue.

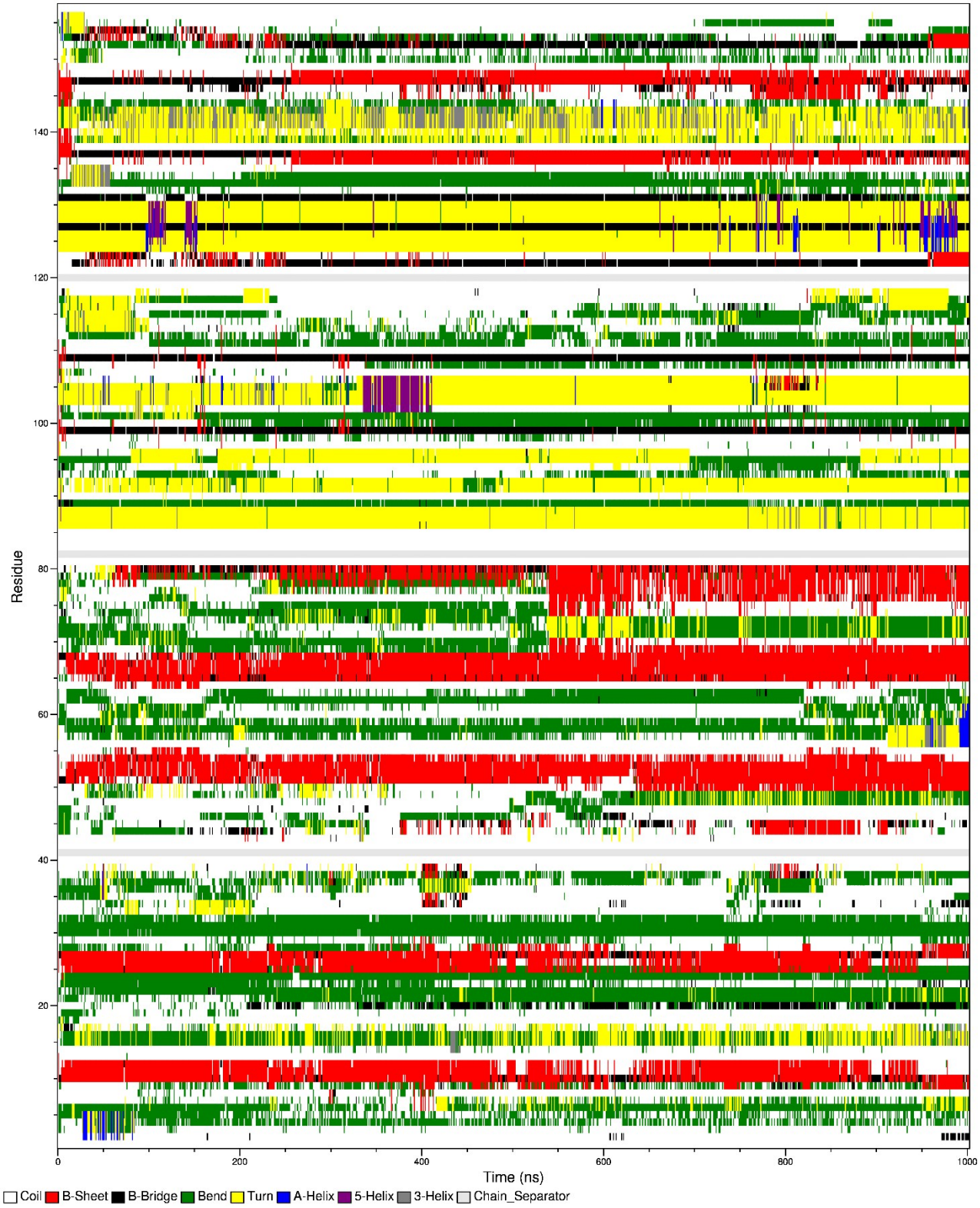
Residue
140
120
100
80
60
40
20
0
200
400
600
800
1000
Time (ns)
Coil
B-Sheet
B-Bridge
Bend
Turn
A-Helix
5-Helix
3-Helix
Chain_Separator

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.

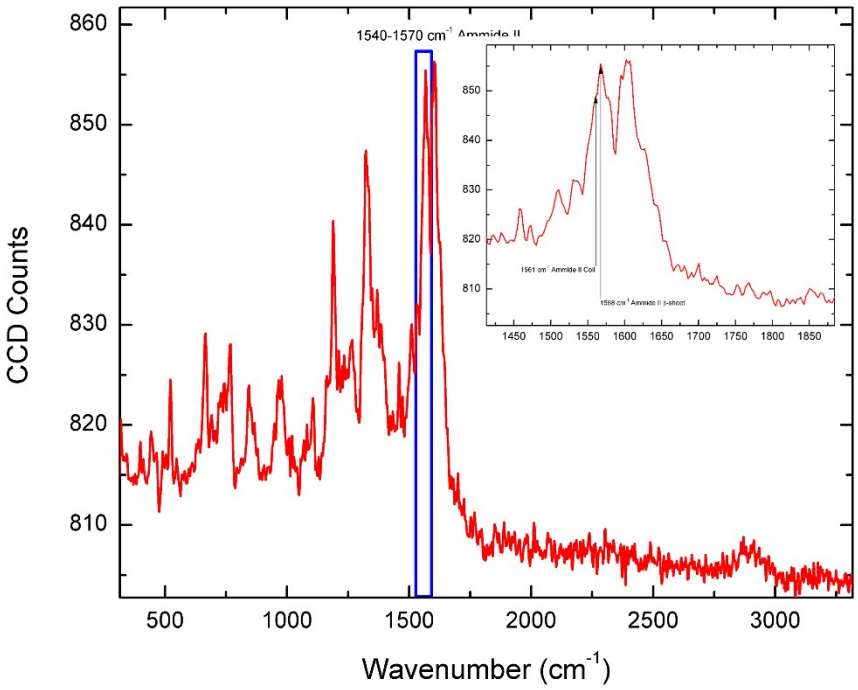

Fig S4. SERS spectra of equimolar mixture of Aβ (1-40) and hIAPP at 10nM concentration. Panel in the right corner is the magnification of the amide II bands. The β-sheet/random coil ratio was calculated from the ratio between the intensity at 1568 cm^{-1}(β-sheet) and intensity at 1561 cm^{-1} (random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