Supplementary Data for

Amyloid β fibrils disruption by oleuropein aglycone: Long-time molecular dynamics simulation to gain insight into the mechanism of action of this polyphenol from extra virgin olive oil

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Figure S1. Timeline representation of the interactions and contacts of Figure 6 in the main text (Hbonds, hydrophobic, ionic, water bridges). Some residues make more than one specific contact with the ligand, which is represented by a darker shade of orange, according to the scale to the right of the plot.



Figure S2. A β fibrils (green cartoon): progression of MD simulation through 5 μ s. The picture was generated by means of PyMOL.



Figure S3. RMSD calculation for each chain of $A\beta$ fibrils without OA.