Supporting Materials

Insights into the effect of Curcumin and (-)-epigallocatechin-3-gallate on the aggregation of Aβ(1-40) monomers by means of molecular dynamics

Francesco Tavanti\textsuperscript{a,b,}\textsuperscript{*}, Alfonso Pedone\textsuperscript{b} and Maria Cristina Menzianib

\textsuperscript{a} CNR-NANO Research Center S3, Via Campi 213/a, 41125 Modena, Italy
\textsuperscript{b} Department of Chemical and Geological Sciences, University of Modena and Reggio Emilia, Via Campi 103, 41125, Modena, Italy

* Correspondence: *To whom correspondence should be addressed. E-mail: francesco.tavanti@nano.cnr.it

\textbf{Figure S 1:} Time evolution of the secondary structure for each residue of the Aβ-amyloid monomeric, dimeric, and trimeric models obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend on the right.
Figure S 2: secondary structure propensity for Aβ monomers interacting with CUR.
Figure S 3: secondary structure propensity for Aβ monomers interacting with EGCG.
Figure S 4: Secondary structure assignment of the single monomer for each residue obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend at the bottom. Monomers + CUR.
Figure S 5: Secondary structure assignment of two monomers for each residue obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend at the bottom. Monomers + CUR
Figure S 6: Secondary structure assignment of three monomers for each residue obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend at the bottom. Monomers + CUR
Figure S 7: Secondary structure assignment of the single monomer for each residue obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend at the bottom. Monomers + EGCG
Figure S 8: Secondary structure assignment of two monomers for each residue obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend at the bottom. Monomers + EGCG
Figure S 9: Secondary structure assignment of three monomers for each residue obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend at the bottom. Monomers + EGCG