Supplementary Information

The anti-amyloidogenic action of Doxycycline: a molecular dynamics study on the interaction with Abeta

Alfonso Gautieri^{a,*}, Marco Gobbi^b, Marten Beeg^b, Federica Rigoldi^a, Laura Colombo^b, Mario Salmona^{b,*}

^a Biomolecular Engineering Lab, Dipartimento di Elettronica, Informazione e Bioingegneria, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano (Italy)

^b Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Via Mario Negri 2, 20156 Milano (Italy)

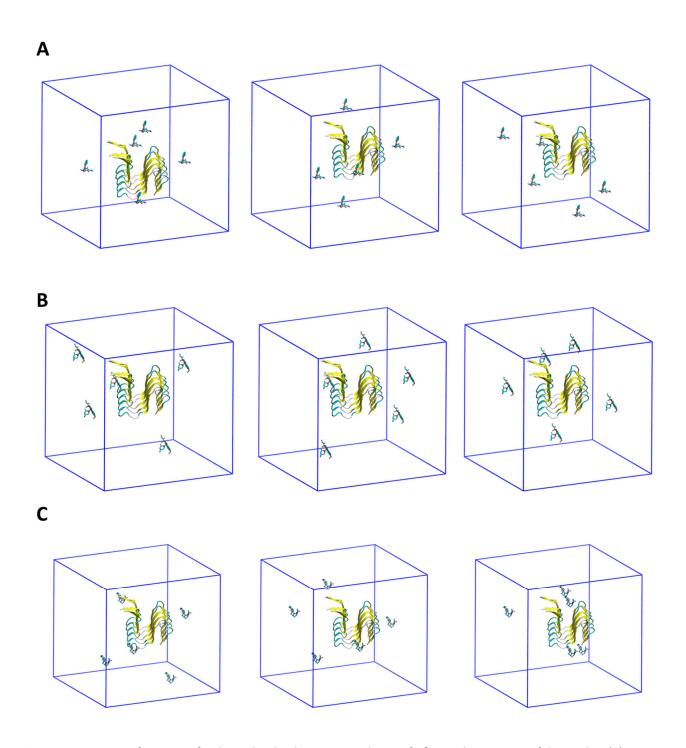
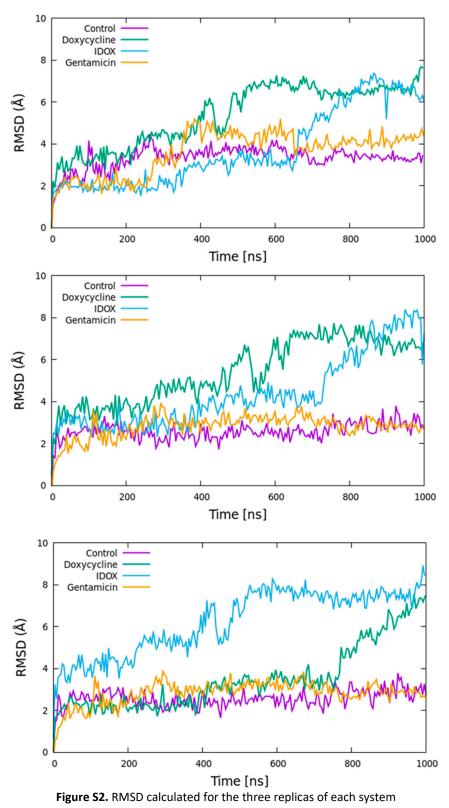


Figure S1. Starting configurations for the molecular dynamics simulation of A β 42 in the presence of doxycycline (A), IDOX (B) and gentamicin (C).



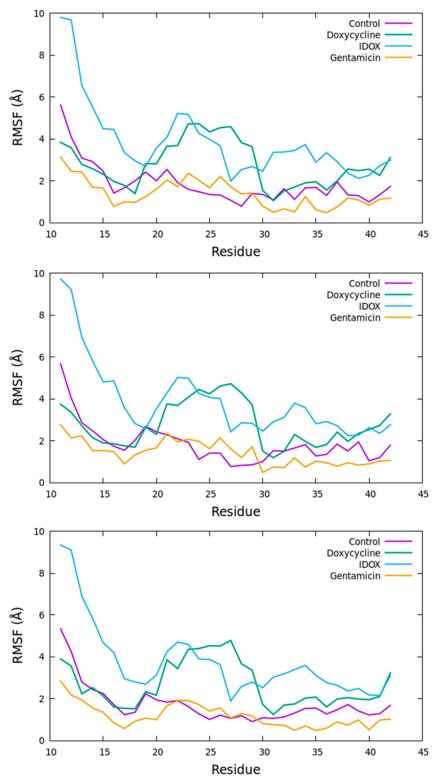


Figure S2. RMSF calculated for the three replicas of each system.