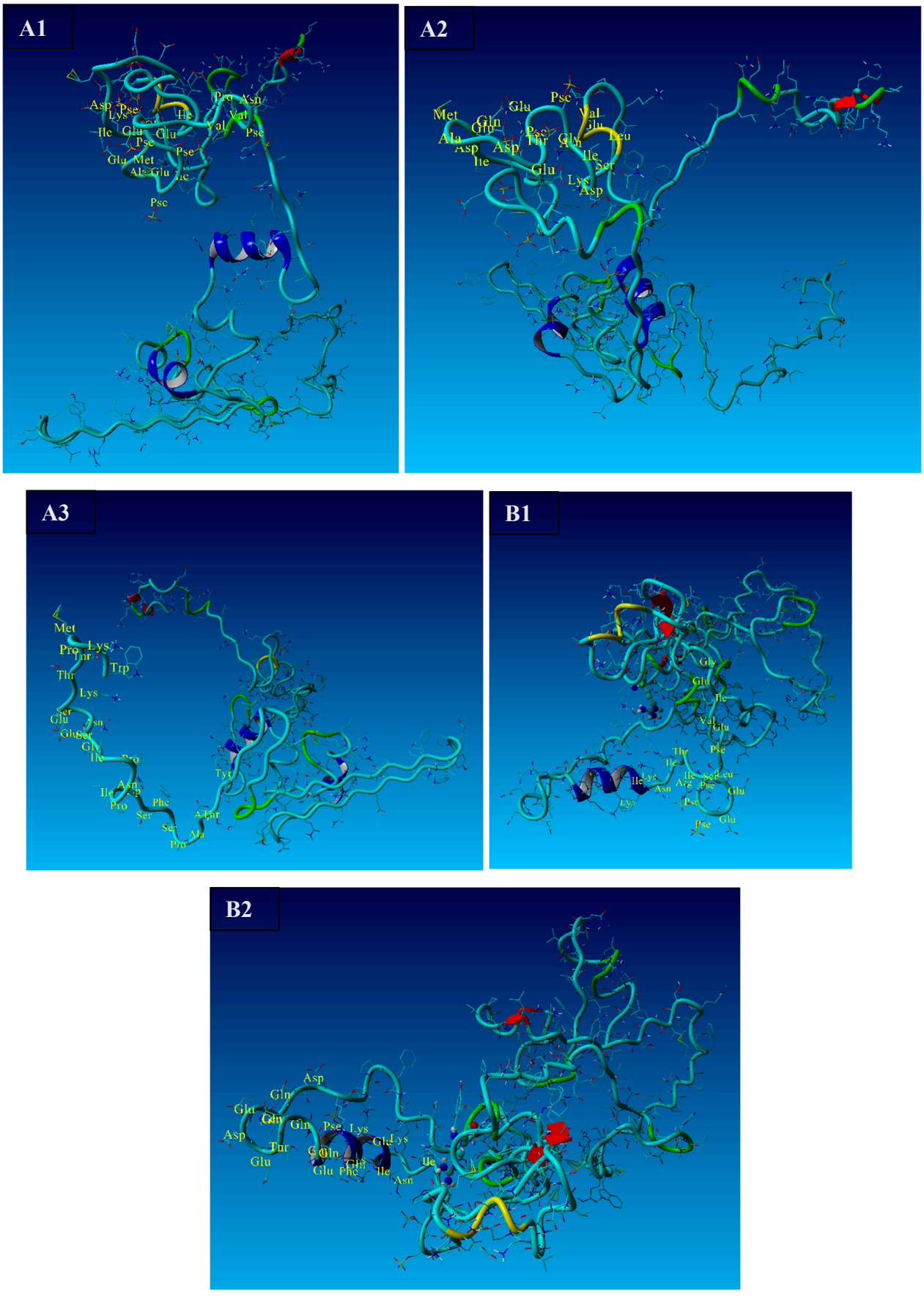


Fig. S1. Illustration of the position of selected aminoacid sequences within α- and β-casein molecule.

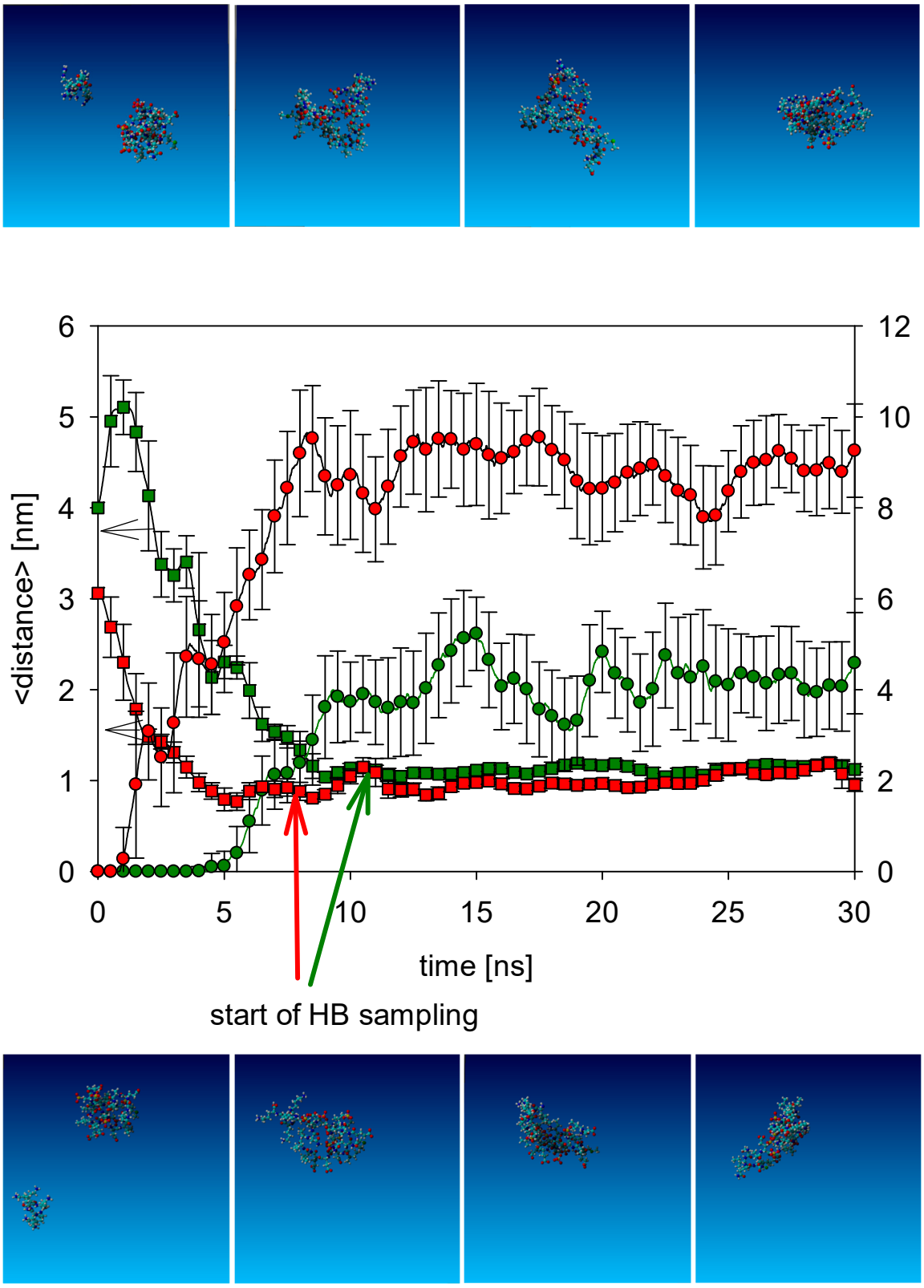


Fig. S2 The example of the evolution of the running average of Seq-A1 sequence-oligomer distance and a number of hydrogen bonds during formation of their aggregate, red symbols for arginine oligomer, green symbols – lysine oligomer. Snapshots from the simulation taken at 0 ns, 5 ns, 20 ns and 30 ns; arginine – above, lysine – below.

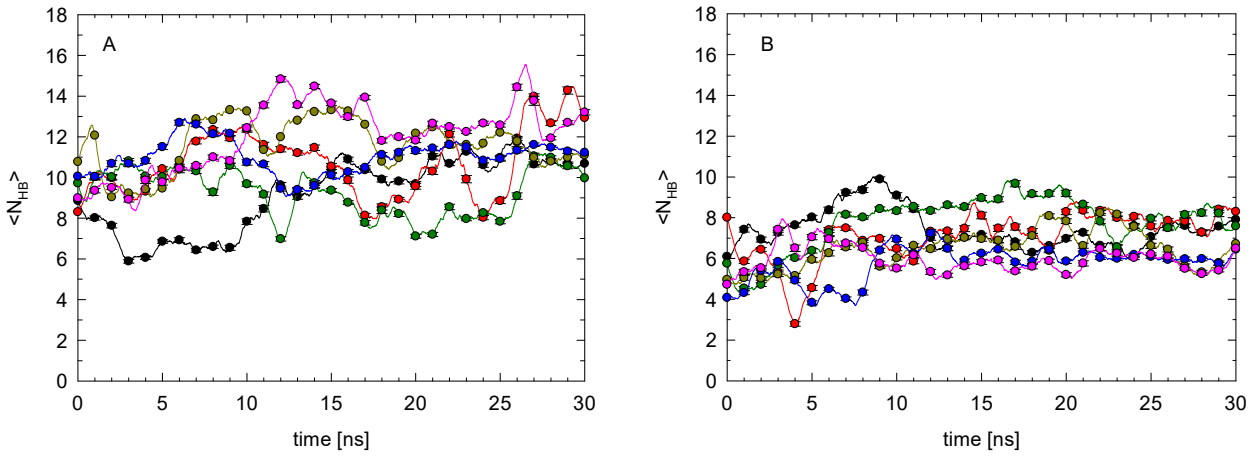
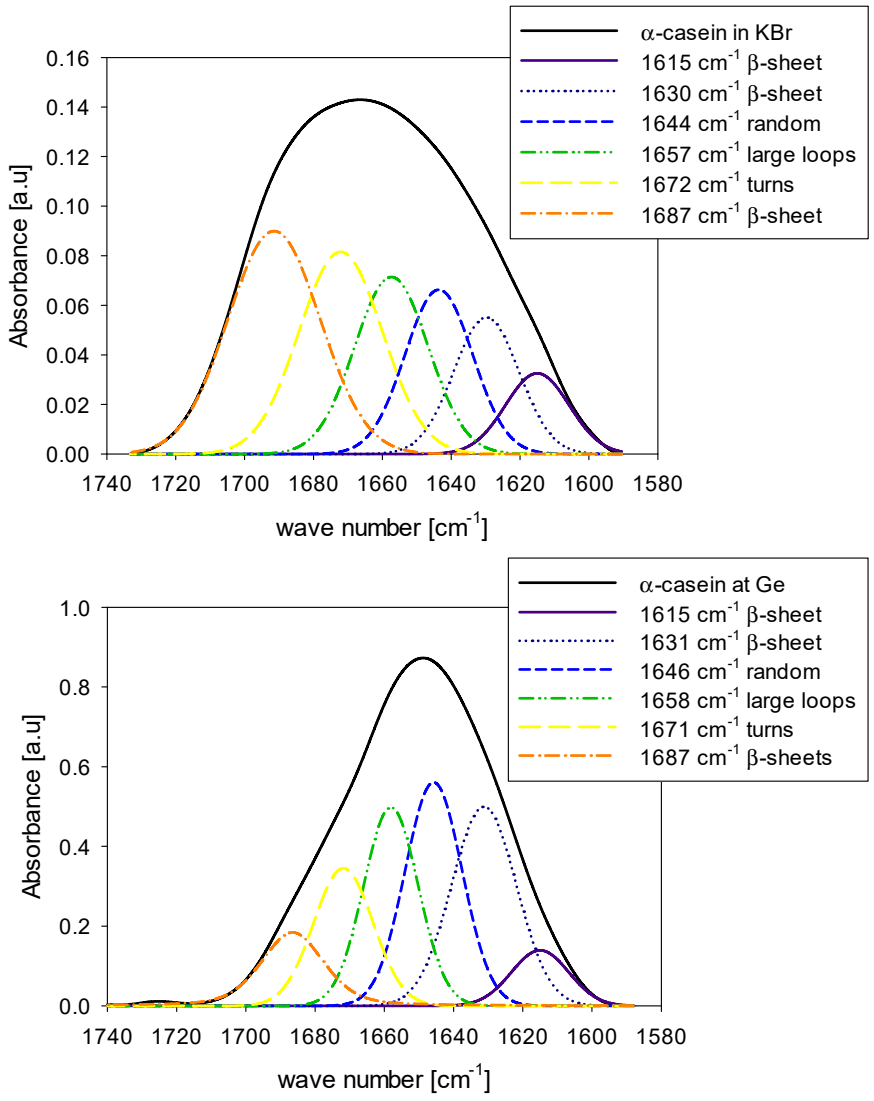


Fig. S3. The evolution of the running average of the number of hydrogen bonds in the Seq-A1 sequence-oligomer aggregates after their formation for six random initial positions. A - Seq-A1-arginine, B - Seq-A1-lysine.



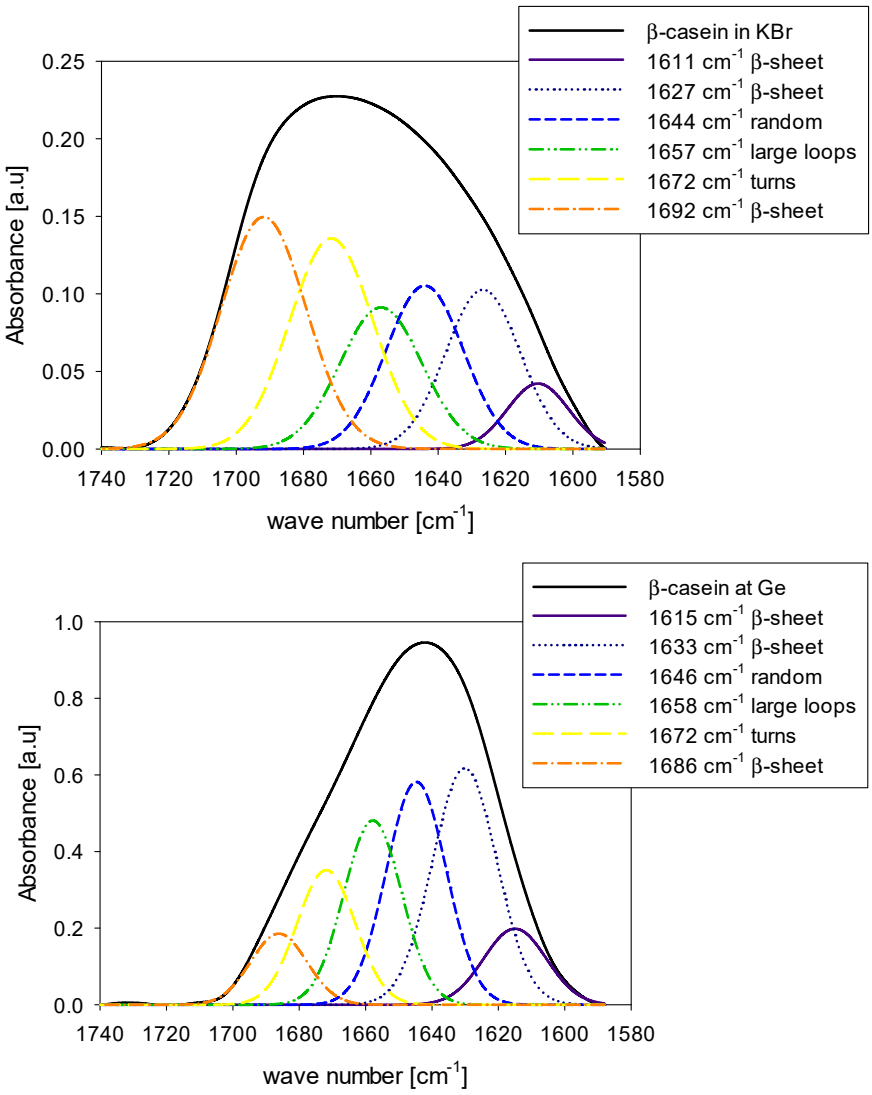


Fig. S4 Decomposition of the amide I band into structural components for α- and β-casein, measured in KBr pellets and in dried film at Ge crystal.

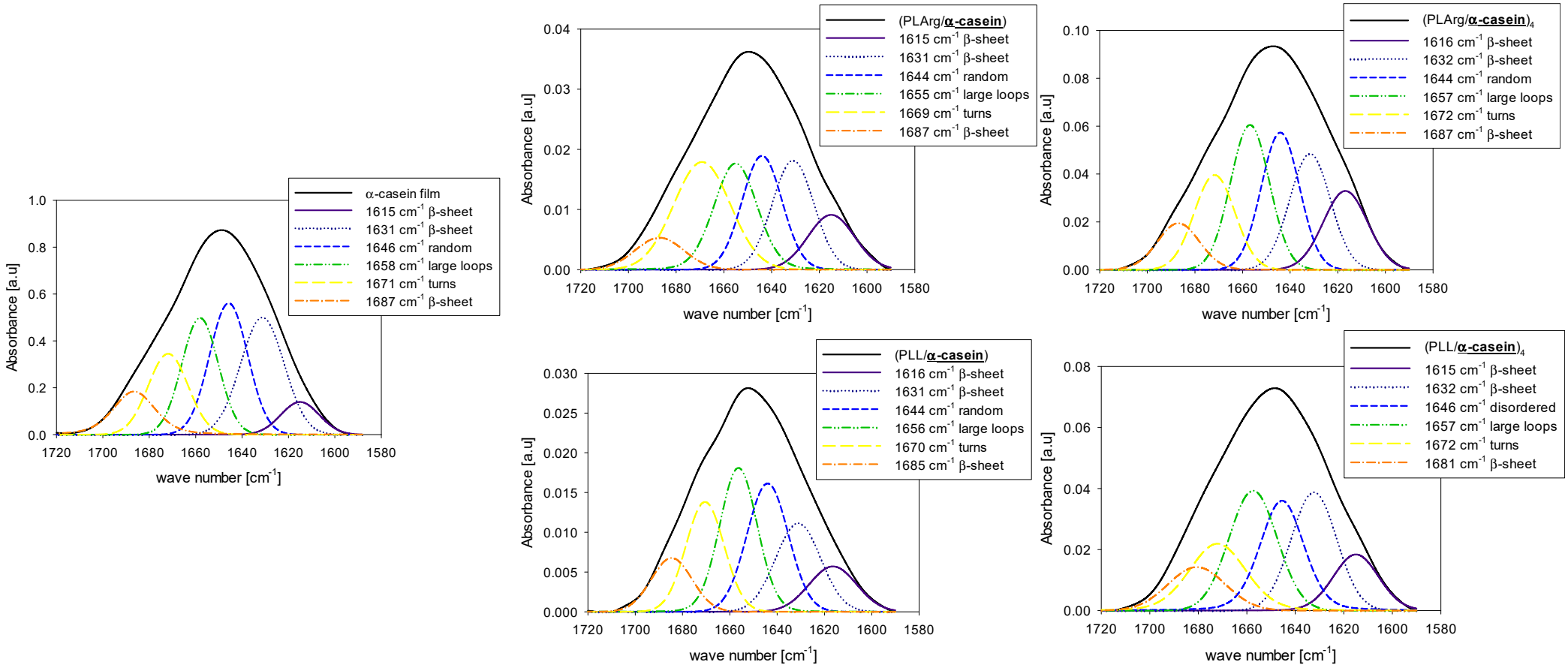


Fig. S5. Decomposition of the amide I band into structural components for α-casein film and the top α-casein layer of (PLArg/α-casein) and (PLArg/α-casein)$_4$ multilayers measured by FTIR ATR at Ge crystal.

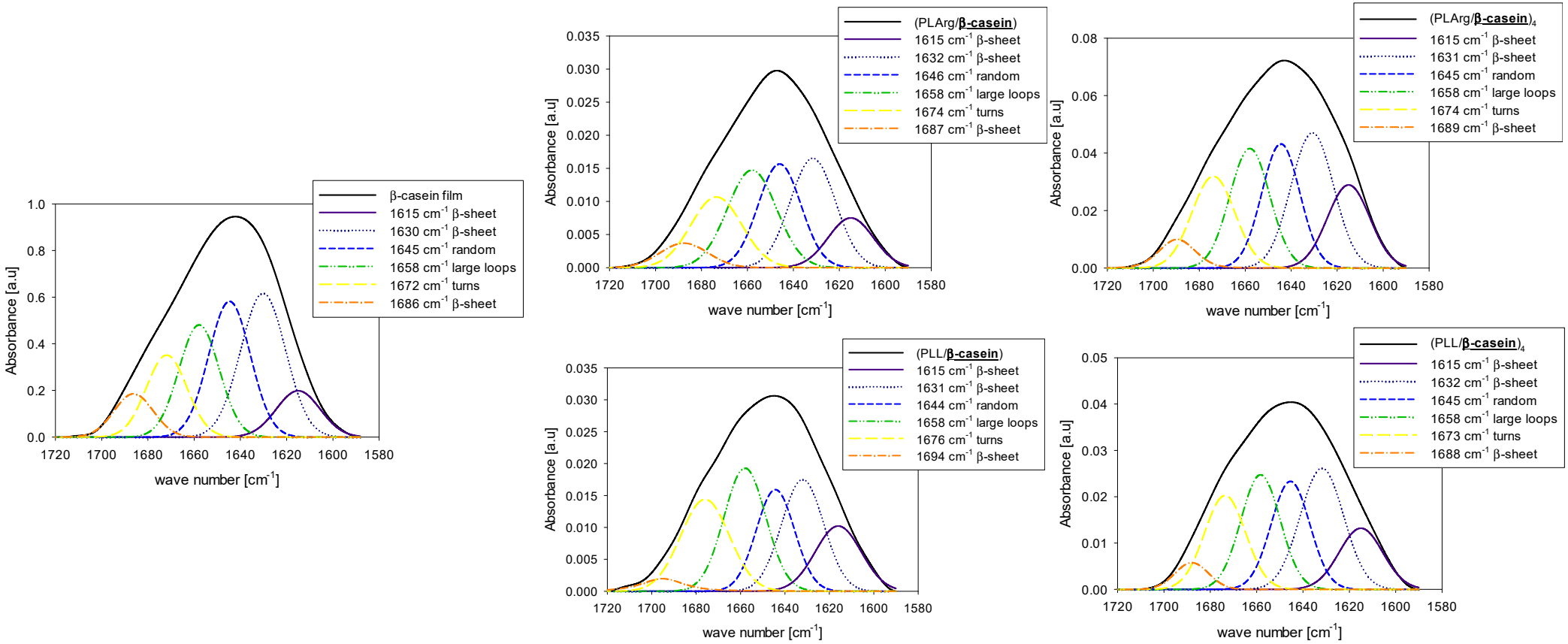


Fig. S6. Decomposition of the amide I band into structural components for β-casein film and the top β-casein layer of (PLArg/β-casein) and (PLArg/β-casein)$_4$ multilayers measured by FTIR ATR at Ge crystal