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# Effect of an unique α-sheet structure on the physicochemical properties and dimerization of IRAK4

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Interleukin-1 receptor-associated kinase 4 (IRAK4), belonging to protein kinase group, is related to Toll-Like Receptor4 (TLR4) signaling in innate immunity. Although IRAK4 inhibitor development researches are active, IRAK4 mutation such as E402x patient indicating deletion from E402 to final residue has immune deficiency disease, causing death. IRAK4 has multiple roles in binding to other signaling proteins as well as protein kinase function. Full-length IRAK4 patients also showed an immune deficiency. In 3D structure view, we identified IRAK4 has an α-sheet structure from D405 to E407 residues. α-sheet suggested by Linus Pauling is polar strand 2nd structure unlike β–sheet structure, same direction amide group and indicating alternating torsion angle (Φ and Ψ) value (+ ↔ –). Amyloid family proteins (Transthyretin or α-synuclein), involved in abnormal structures, misfolding and aggregation was reported as including α-sheet structures by molecular dynamics (MD) simulation. Other structural properties related to α-sheet were also studied in ion-channels conducting $K^+$ ion as well as amyloid protein concerned with protein aggregation. In addition to MD simulation structures, many protein crystal structures are being released in Protein Data Bank (PDB) nowadays by improved crystallization technics. α-sheet identification using recent all PDB showed that IRAK4 has α-sheet structure. In this study, how identified IRAK4 as an α-sheet structure is related to physicochemical properties in protein-protein interaction, stability and solvation was interested. For more detail structure researches of IRAK4, crystal structures using not one PDB but all PDBs were analyzed calculating torsion angle, distance and salvation. Furthermore, MD simulation structures including both monomer and dimer were analyzed depending on each trajectory. This research for IRAK4 relating to the α-sheet structure may establish new insight as well as structural properties of previous amyloid proteins and ion channel related to α-sheet.

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