

Structure of Mimotopes Recognized by the Monoclonal Antibodies against anti Apolipoprotein A-I

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Apolipoprotein A-I (Apo-AI) is a major protein component for high density lipoprotein(HDL) and is responsible for the clearance of cholesterol from the blood. A number of mimetic peptides of apolipoproteins were screened from the phage-displayed random peptide library by utilizing monoclonal antibody against the Apo-AI. Conformational studies for two mimetic peptides CPFARLPVEHHDVVGL (pA1) and FVLVRDTPSSVCCP (pA2) recognized by the monoclonal antibodies will be discussed in this study. NMR signal assignments were accomplished by using homo/heteronuclear 2D-NMR techniques. Temperature-dependent with five different NOE mixing times(10, 50, 100, 300, 500 ms) NOESY experiments were made for structure determination and 2D-NOE back-calculations. NOE volume integrations were made by using HyNMR and subsequently assessed to the molecular dynamic computations. Solution-state structures of these mimotopes were determined by using NMR methods and NMR-based distance geometry (DG)/molecular dynamic(MD) computations. Structures were generated with loose NOE-derived interproton distance restraints (2.0-2.5 Å, 2.0-3.5 Å and 2.0-4.5 Å for strong, medium, and weak NOE cross-peak intensities, respectively), and 2D NOESY back-calculations of structures were carried out for establishing the consistency between experimental data and dynamic structures.