Poster Presentation

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A comparative analysis on x-ray structure of cobalamin binding proteins

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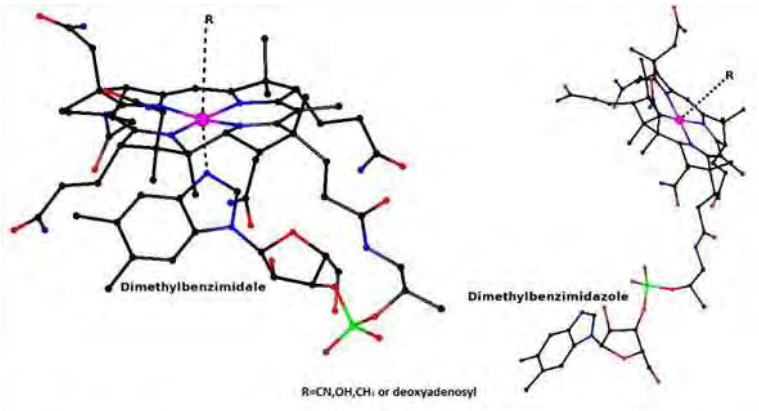
Vitamin B12 (Cobalamin;Cbl;B12; Figure) is a water soluble vitamin and is an essential component for the growth and development of many eukaryotes and prokaryotes organisms. B12 coordinates a cobalt ion in the center of the ring through the four pyrrole nitrogen atoms, the fifth ligand is dimethylbenzimidazole (DMB) moiety and the sixth ligand can be methyl group, deoxyadenosyl, cyanide or OH-. The structurally diverse groups of B12 binding proteins involved in various important biological functions. B12 adopts either base-on or base-off conformation in B12 binding proteins (Figure). An in-depth analysis on these structures was carried out using PDB coordinates (www.pdb.org) of a carefully chosen database of B12 binding proteins to correlate the overall folding of the molecule with phylogeny, the B12 interactions, and with biological function. The chosen database can be divided into three distinct groups. The first group is B12 transport proteins in mammals and the second is B12 transport proteins in E.Coli. The third group can be broadly clarified as B12-dependent enzymes. Results: The molecular architecture of the B12 binding proteins is diverse. It varies from a two-domain to multi-domain proteins. An analysis on the environment around B12 molecule shows that hydrogen bonds or vander waals interactions are dominant interactions between B12 and protein. Both conventional hydrogen bonds (N-H….X and O-H….X) and weak C-H….X hydrogen bonds play important role in these interactions. The number of protein residues interacting with B12 varies widely from 2 to 18 residues, depending on the nature of biological function. The analysis clearly establishes that B12 is amazingly adoptive to wide range of environments, namely polar, non-polar or charged. The B12 uses its functional groups both at head, corrin ring and in tail region (phosphate or DMB groups) at optimum level to form stable complex with partner proteins. Details will be presented.

[1] *Sukumar, N. (2013) Biochimie, 95, 976-988.,* ***[2]*** *Sukumar, N., Mathews, F.S., Gordon, M.M., Ealick, S.E. & Alpers, D.H. (2009) Cryst. Growth. Des. 9, 348-351.,* ***[3]*** *Mathews, F.S., Gordon, M.M., Chen, Z., Rajashankar, K.R., Ealick, S.E., Alpers, D.H. & Sukumar, N. (2007) Proc. Natl. Acad. Sci. USA., 104, 17311-17316.*



B12 conformation in cobalamin binding proteins. B12 can adopt base-on (left) and base-off (right) conformation

Keywords: vitamin B12, membrane protein, transport protein