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Hydration of Protein-RNA Recognition Sites

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Abstract : We investigate the role of water molecules in 89 protein-RNA complexes taken from the Protein Data Bank. Those with tRNA and single-stranded RNA are less hydrated than with duplex or ribosomal proteins. Protein-RNA interfaces are hydrated less than protein-DNA interfaces, but more than protein-protein interfaces. Majority of the waters at protein-RNA interfaces makes multiple H-bonds; however, a fraction does not make any. Those making Hbonds have preferences for the polar groups of RNA than its partner protein. The spatial distribution of waters makes interfaces with ribosomal proteins and single-stranded RNA relatively 'dry' than interfaces with tRNA and duplex RNA. In contrast to protein-DNA interfaces, mainly due to the presence of the 2'OH, the ribose in protein-RNA interfaces is hydrated more than the phosphate or the bases. The minor groove in protein-RNA interfaces is hydrated more than the major groove, while in protein-DNA interfaces it is reverse. The strands make the highest number of water-mediated H-bonds per unit interface area followed by the helices and the non-regular structures. The preserved waters at protein-RNA interfaces make higher number of H-bonds than the other waters. Preserved waters contribute toward the affinity in protein-RNA recognition and should be carefully treated while engineering protein-RNA interfaces.

Keywords : h-bonds, minor-major grooves, preserved water, protein-RNA interfaces
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