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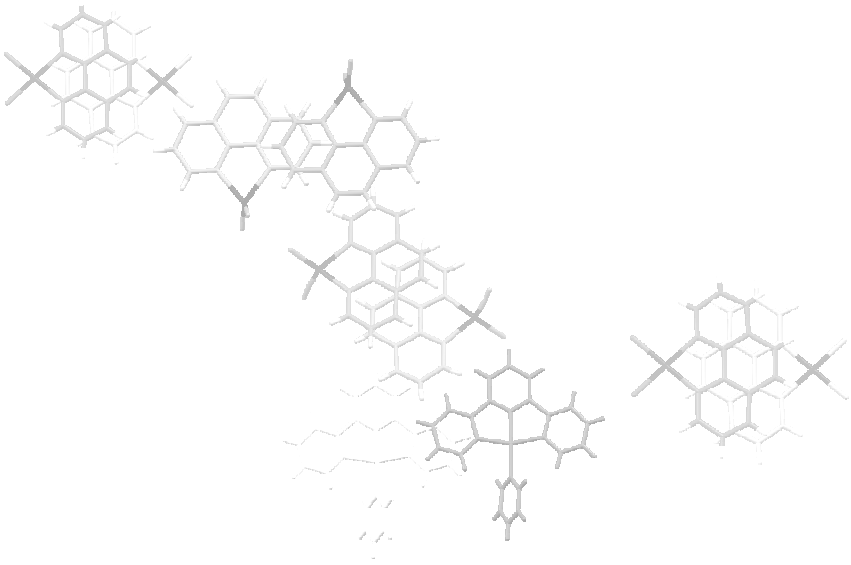

BOOK OF ABSTRACTS

Identification of Hot spots in Sm protein interfaces

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The Sm family of proteins are closely associated with RNA metabolism throughout all of life. These proteins form homomorphic and heteromorphic rings consisting of six or seven subunits with a characteristic central pore, the presence of which is critical for binding U-rich regions of single-stranded RNA. This study aims to characterize the interface hot spot residues of subunits in Sm proteins. We performed an analysis of the X ray structure of 15 Sm motif containing proteins from the Protein Data Bank (PDB) and summarize physicochemical properties in an effort to understand the origin of their stabilizing contributions to protein–protein associations.

Homo-oligomer interfaces have greater number of interface residues and hydrophobic residues (Ala, Val, Leu, Met, Ile, Phe) are predominant at the homo-oligomer interfaces. However, the study shows that charged residues (Asp, Glu, Lys, Arg) and hydrophilic residues (Asn, Thr, Ser, Gln, His, Trp, Tyr) are dominant at the hetero-oligomer interfaces. Analysis of amino acid enrichment in hot spots shows that some residues are more favorable. The most frequent ones, Met, Arg, Pro, Thr and Tyr, are critical due to their capability of making multiple types of favorable interactions and lowered effective dielectric environment of hot spots.

Our results show that low relCompASA is critical for a residue to be a hot spot. Though many of the hot spot residues have similar relCompASA values with nonhot spot residues, they have different mean values (hot spots: 5.1%, non-hot spots: 29.1%). The *P*-value for relCompASA is less than 0.05, which indicate that hot spots located near the center of the interface are a general property of the interfaces, and largely protected from bulk solvent (corresponding to low relCompASA). RelΔASA indicates the change in the solvent accessibility of a residue, and correlate significantly with relCompASA. Additionally, knowledge-based pair potentials of residues is statistically significant to discriminate hot spots and non-hot spots (P-value = 5.7×10^{-6}). These results indicate that hot spots are mostly buried, tightly packed and form a network of favorable interactions with other residues.

Structurally conserved residues and hot spots correlate significantly, and demonstrate that hot spots play an important role in the stability of oligomers.