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Bayesian Secondary Structure Assignment of Human Activating Signal Co-integrator 1 Complex Subunit 2 (ASCC2): Structural Architecture for Somatic Cancer Prophylaxis and Therapy

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The human genome experiences a constant threat due to deoxyribonucleic acid (DNA) damaging agents unwittingly leading to somatic cancer mutations. Cell level evolutions have developed functional units to recognize DNA damages and to devise mechanisms for DNA repairs. This is highly advantageous in preventing risks leading to somatic cellular mutations and cancers. The DNA repair mechanisms involving human activating signal co-integrator complex (ASCC) are highlighted in many enzyme-mediated repairs, especially AlkBH3-mediated DNA repair. Among four subunits of the ASCC (ASCC1, ASCC2, ASCC3 and ASC1/TRIP4), ASCC2 is ultimately poignant in signaling and repairing for the instances of DNA alkylation damages. ASCC2-ASCC3 complex is widely recognized in the DNA repair mechanisms and experimental investigations have raised concerns around precise interacting regions of these two subunits. Structural knowledge of the complex is essential in figuring out molecular mechanisms and is widely lacking. To better appreciate this interaction, a computational structural informatics analysis of the ASCC2 is carried out at the secondary level employing Bayesian statistical inference of minimum message length (MML). Secondary structure (SST) segmentations (SEGs), SST assignment and secondary structural elements (SSEs) are computed for the input coordinate data of the ASCC2. The right-handed α helix type is observed to be frequently occurring in the sequence. Nine distinguished segment indices are identified upon computing. Segment index 3 of chain A is found to be right/ left-handed α-like helix. All the four different secondary structural elements of the human ASCC2 identified in this work correspond to a common H type with variation in the number of residues. Overall, the present informatics study is aimed to further investigate joint conformation of the ASCC2-ASCC3 complex in the light of establishing promising prophylaxis and treatment.

Keywords: *ASCC2, secondary structure, DNA repair, structural informatics, Bayesian method*